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(54) **ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES**

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Related U.S. Application Data

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H01L 51/00 (2006.01)
(Continued)

(52) **U.S. Cl.**
CPC ***H01L 51/0094*** (2013.01); ***C07F 7/0816*** (2013.01); ***C07F 15/0033*** (2013.01);
(Continued)

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CPC H01L 51/0084–51/0092; H01L 51/50; H01L 51/5012; H01L 51/5016; H01L 51/5048; H01L 51/5056; H01L 51/5072; H01L 51/0094; C07F 7/0816; C07F 15/0086; C07F 15/0033; C07F 7/081; C07F 7/082; C07F 7/0836; C09K 11/06; C09K 2211/1007; C09K 2211/1011; C09K 2211/1029; C09K 2211/104; C09K 2211/1044; C09K 2211/1059; C09K 2211/1092
USPC 428/690, 917; 313/504, 505, 506; 257/40, E51.024, E51.025, E51.026, 257/E51.041, E51.043, E51.044; 556/407; 526/241, 279; 528/38, 395, 423
See application file for complete search history.

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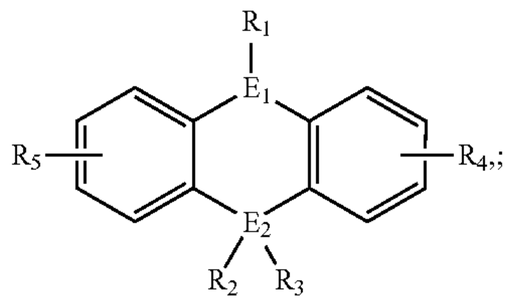
(57) **ABSTRACT**

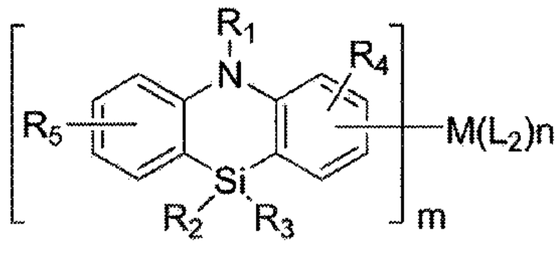
A phenazasiline comprising compound, and devices and formulations including the same are described. The compound includes a ligand L_1 including:

Formula I



wherein E_1 is N, E_2 is Si, and R_4 and R_5 represent mono, di, tri, tetra substitutions or no substitution;
wherein R_1, R_2, R_3, R_4, and R_5 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, and any two adjacent R_1, R_2, R_3, R_4, and R_5, are optionally joined to form a ring, which may be further substituted. In Formula I, L_1 is coordinated to metal M, which has an atomic weight higher than 40, provided that the metal M does not form bond with E_1 and E_2. L_1 may be linked with other ligands.

33 Claims, 3 Drawing Sheets



Formula II

(51) **Int. Cl.**

C07F 15/00	(2006.01)
C07F 7/08	(2006.01)
C09K 11/06	(2006.01)

(52) **U.S. Cl.**

CPC ***C07F15/0086*** (2013.01); ***C09K 11/06*** (2013.01); ***H01L 51/0085*** (2013.01); *C09K 2211/104* (2013.01); *C09K 2211/1007* (2013.01); *C09K 2211/1011* (2013.01); *C09K 2211/1029* (2013.01); *C09K 2211/1044* (2013.01); *C09K 2211/1059* (2013.01); *C09K 2211/1092* (2013.01); *C09K 2211/185* (2013.01); *H01L 51/5016* (2013.01)

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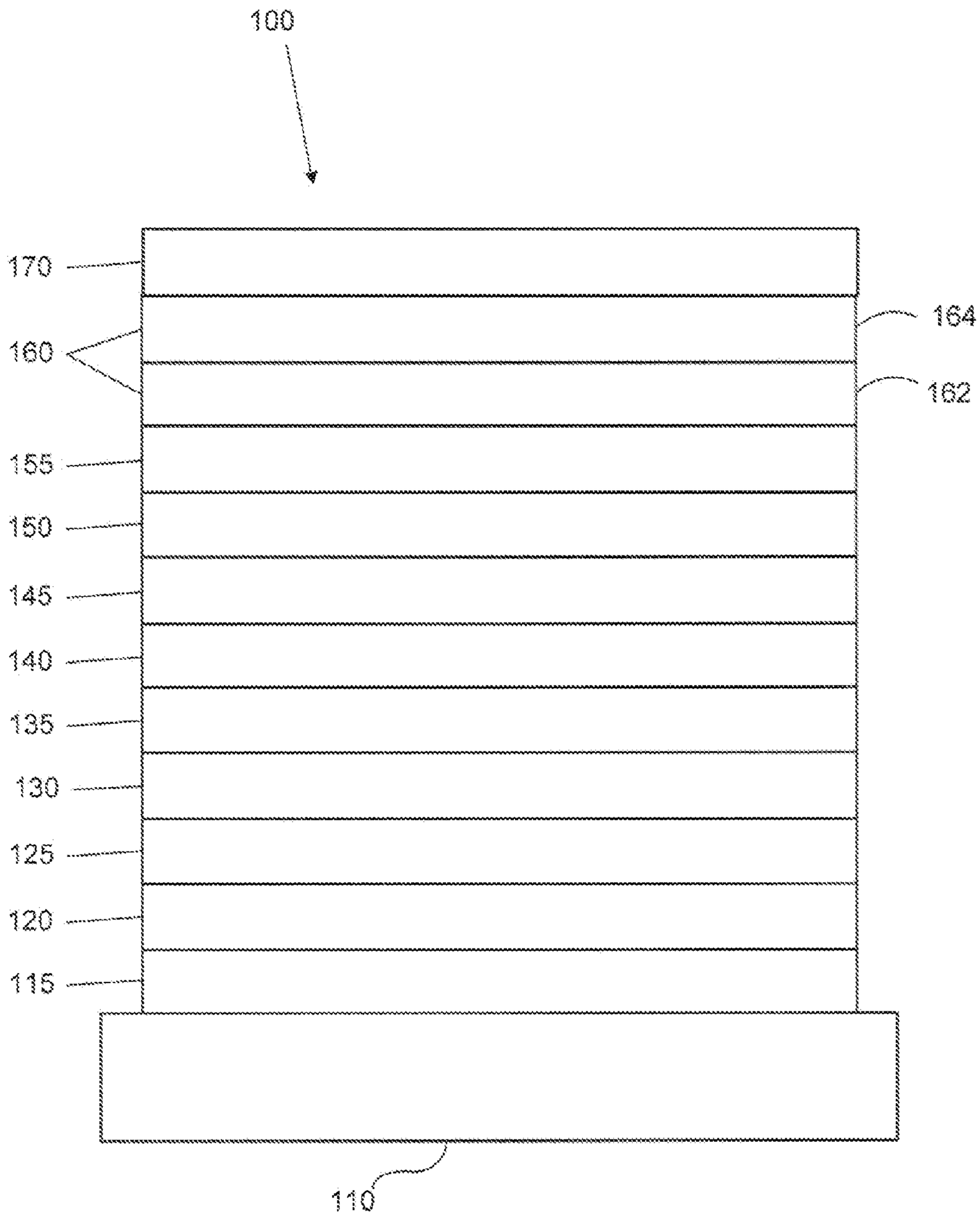


FIGURE 1

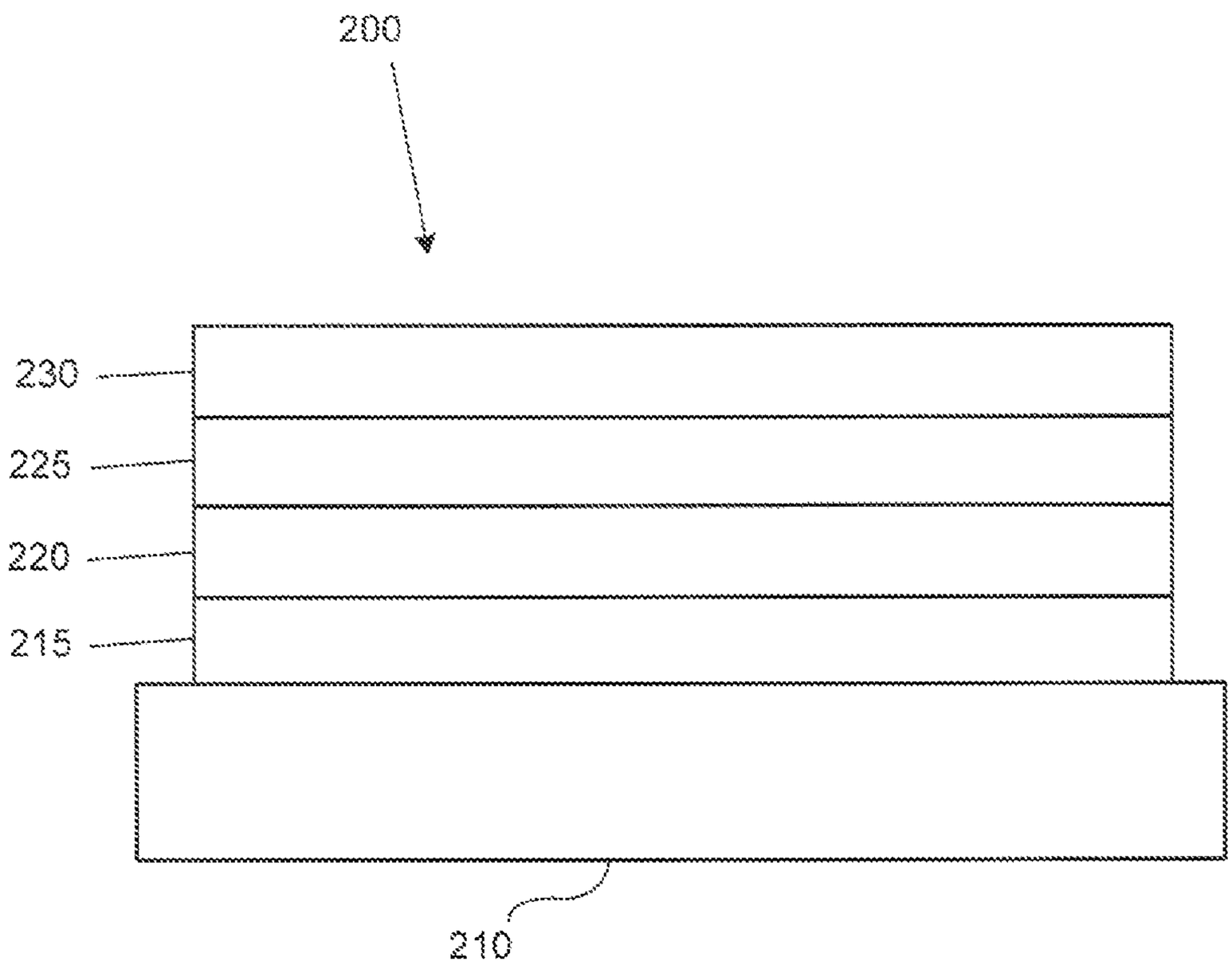


FIGURE 2

Formula I

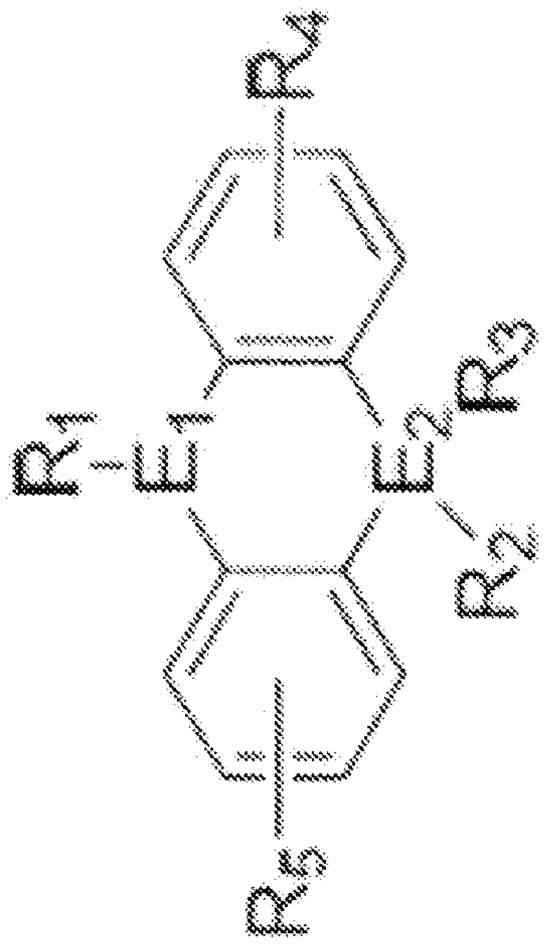


Figure 3

Formula II

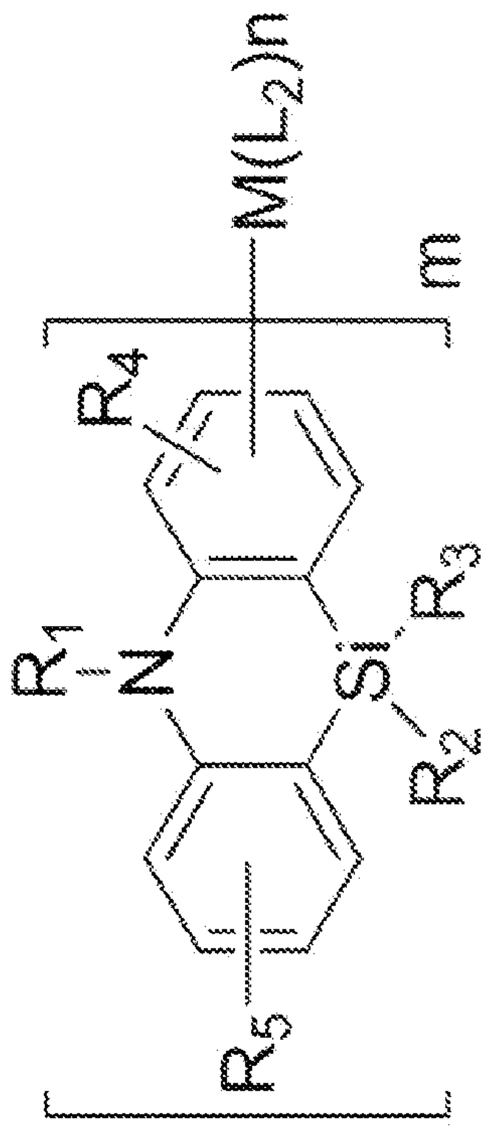


Figure 4

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application Ser. No. 61/662,617 filed Jun. 21, 2012, the entire content of which is incorporated herein by reference.

PARTIES TO A JOINT RESEARCH AGREEMENT

The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: Regents of the University of Michigan, Princeton University, University of Southern California, and the Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

FIELD OF THE INVENTION

The present invention relates to compounds for use as emitters and devices, such as organic light emitting diodes, including the same.

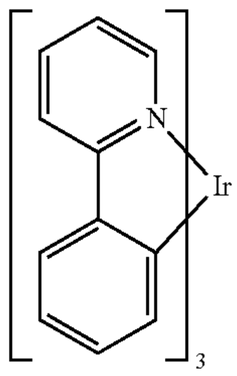
BACKGROUND

Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Color may be measured using CIE coordinates, which are well known to the art.

One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted $Ir(ppy)_3$, which has the following structure:



In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.

As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

As used herein, "solution processable" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level of the same material. A "higher"

HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

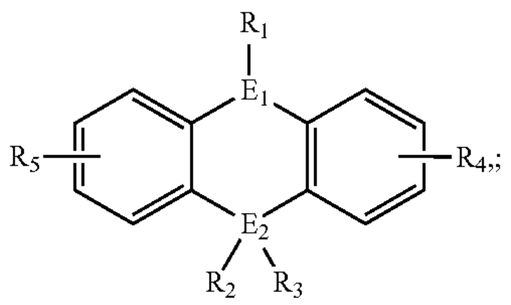
As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

SUMMARY OF THE INVENTION

According to an embodiment, a compound is provided that includes a ligand L_1, wherein L_1 comprises the following formula:

Formula I



wherein E_1 is N; E_2 is Si; R_4 and R_5 represent mono, di, tri, tetra substitutions or no substitution; and R_1, R_2, R_3, R_4, and R_5 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; wherein any two adjacent R_1, R_2, R_3, R_4, and R_5 can be optionally joined to form a ring, which may be further substituted. L_1 is coordinated to the metal M, which has an atomic weight higher than 40, provided that the metal M does not form bond with E_1 and E_2. L_1 may be linked with other ligands to comprise a bidentate, tridentate, tetradentate, pentadentate or hexadentate ligand.

According to another embodiment, a first device comprising a first organic light emitting device is also provided. The first device can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer includes a compound including ligand L_1 coordinated to the metal M. The first device can be a consumer product, an organic light-emitting device, and/or a lighting panel.

According to still another embodiment, a formulation that includes ligand L_1 coordinated to the metal M is provided.

BRIEF DESCRIPTION OF THE DRAWINGS

The present disclosure is best understood from the following detailed description when read in conjunction with the accompanying drawing. It is emphasized that, according to common practice, the various features of the drawing are not necessarily to scale. On the contrary, the dimensions of the various features are arbitrarily expanded or reduced for clarity. Like numerals denote like features throughout the specification and drawings.

FIG. **1** shows an organic light emitting device.

FIG. **2** shows an inverted organic light emitting device that does not have a separate electron transport layer.

FIG. **3** shows Formula I as disclosed herein.

FIG. **4** shows Formula II as disclosed herein.

DETAILED DESCRIPTION

Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-1") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

FIG. **1** shows an organic light emitting device **100**. The figures are not necessarily drawn to scale. Device **100** may include a substrate **110**, an anode **115**, a hole injection layer **120**, a hole transport layer **125**, an electron blocking layer **130**, an emissive layer **135**, a hole blocking layer **140**, an electron transport layer **145**, an electron injection layer **150**, a protective layer **155**, a cathode **160**, and a barrier layer **170**. Cathode **160** is a compound cathode having a first conductive layer **162** and a second conductive layer **164**. Device **100** may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F_4-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its

entirety. An example of an n-doped electron transport layer is BPhen doped with L_1 at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

FIG. **2** shows an inverted OLED **200**. The device includes a substrate **210**, a cathode **215**, an emissive layer **220**, a hole transport layer **225**, and an anode **230**. Device **200** may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device **200** has cathode **215** disposed under anode **230**, device **200** may be referred to as an "inverted" OLED. Materials similar to those described with respect to device **100** may be used in the corresponding layers of device **200**. FIG. **2** provides one example of how some layers may be omitted from the structure of device **100**.

The simple layered structure illustrated in FIGS. **1** and **2** is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device **200**, hole transport layer **225** transports holes and injects holes into emissive layer **220**, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. **1** and **2**.

Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. **1** and **2**. For example, the substrate may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processability than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material consists essentially of polymeric silicon and inorganic silicon.

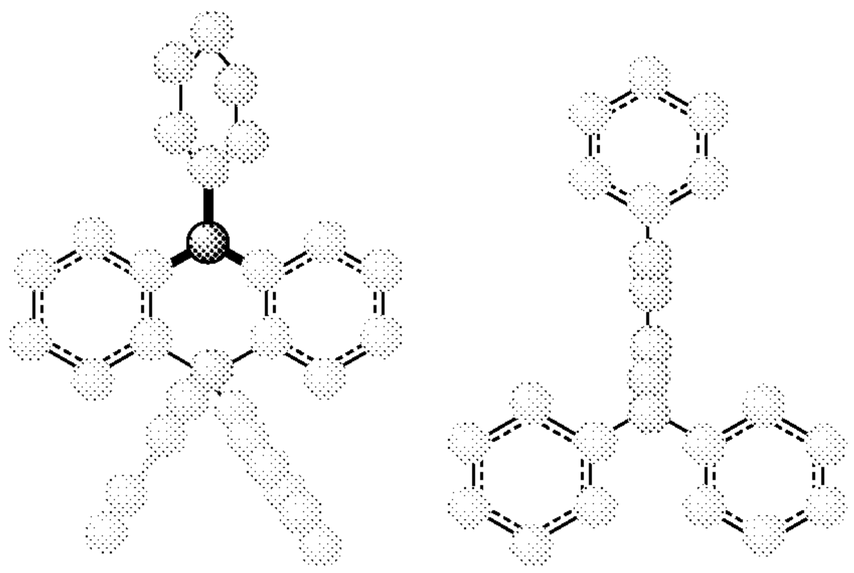
Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders, viewfinders, micro-displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.).

The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

The terms halo, halogen, alkyl, cycloalkyl, alkenyl, alkynyl, arylkyl, heterocyclic group, aryl, alkylaryl, aromatic group, and heteroaryl are known to the art, and are defined in U.S. Pat. No. 7,279,704 at cols. 31-32, which are incorporated herein by reference.

As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant carbon. Thus, where R^2 is monosubstituted, then one R^2 must be other than H. Similarly, where R^3 is disubstituted, the two of R^3 must be other than H. Similarly, where R^2 is unsubstituted R^2 is hydrogen for all available positions.

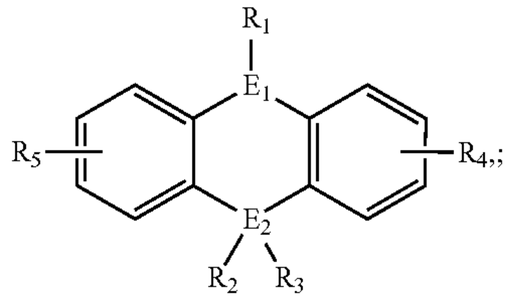
According to an embodiment, metal-phenazasilin complexes are provided that may be useful as emitters when incorporated into OLED devices. Substituted dihydrodibenzo[b,e][1,4]azasiline, or phenazasilin, compounds have been used as host or hole transporting materials in OLEDs. The tetrahdral geometry around silicon normally decreased solid state packing, resulting in amorphous materials. As show in the 3D structures of 5,10,10-triphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (below), the phenyl ring on nitrogen atom (top position of central ring) is perpendicular to the phenazasilin ring.



This feature, together with the phenyl groups on silicon (bottom position on central ring), further prevents π-π stacking in solid state. It may be beneficial to introduce phenazasilin groups into phosphorescent metal complexes to achieve high PL quantum yield through decreased solid state packing. In addition, the multiple fused ring structure provides rigidity to the ligand. It is known that rigidifying ligands in metal complexes can narrow the emission spectra. It is often desirable to have narrow emission spectra to achieve more saturated colors in OLED devices. Therefore, phosphorescent metal complexes bearing ligands with phenazasilin structures, such as those described herein, may provide more saturated colors.

According to one embodiment, a compound that include a ligand L1 coordinated to a metal M, which has an atomic weight higher than 40, is described. The ligand L_1 can include the following formula:

Formula I



wherein E_1 is N;

wherein E_2 is Si;

wherein R_4 and R_5 represent mono, di, tri, tetra substitutions or no substitution;

wherein R_1, R_2, R_3, R_4, and R_5 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

wherein any two adjacent R_1, R_2, R_3, R_4, and R_5 are optionally joined to form a ring, which may be further substituted;

wherein metal M does not form bond with E_1 and E_2; and

wherein L_1 may be linked with other ligands to comprise a bidentate, tridentate, tetradentate, pentadentate or hexadentate ligand.

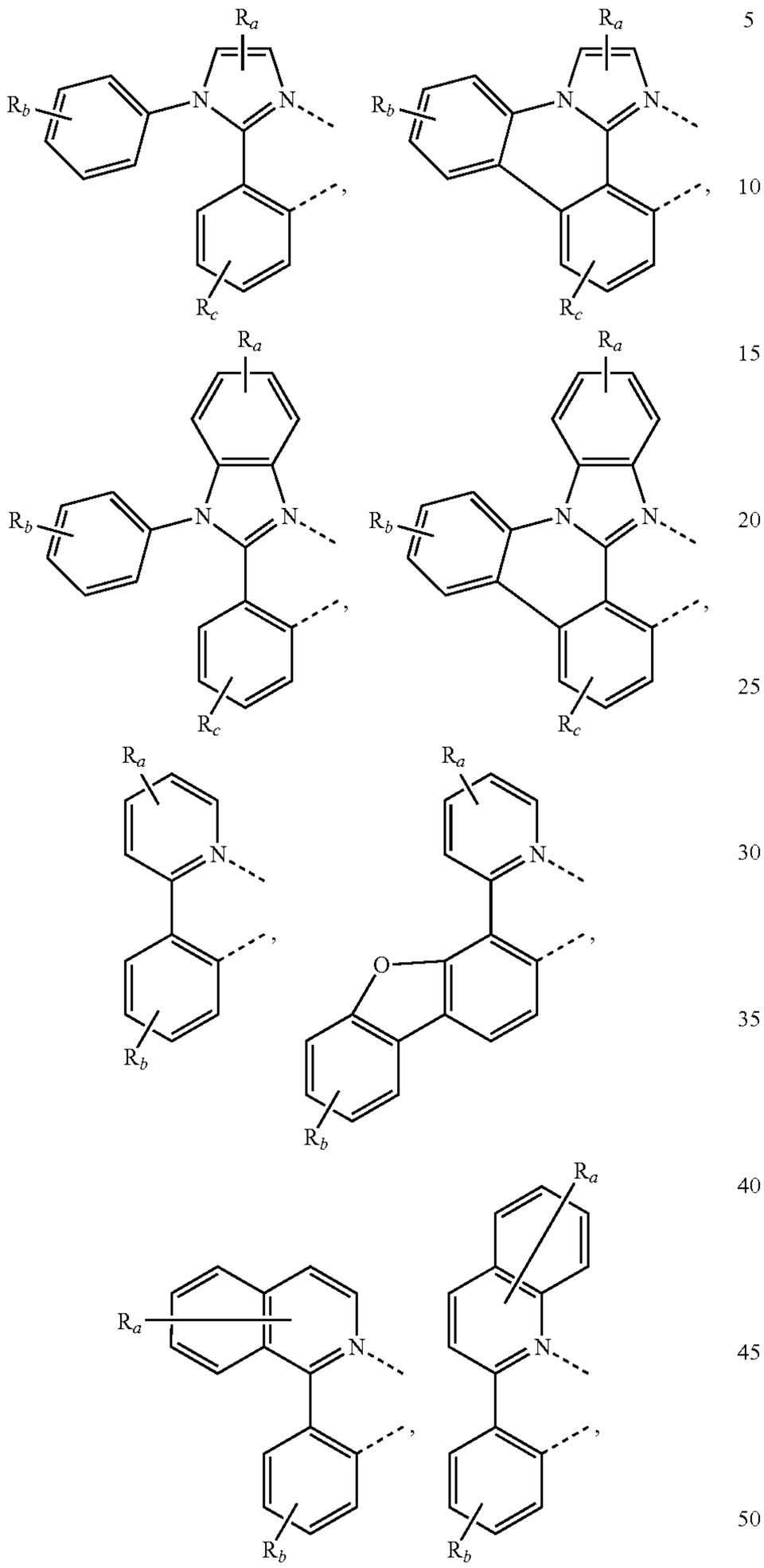
The metal M can be selected from the group consisting of Ir, Pt, Re, Os, Ru, Rh, Pd, Cu, Ag, and Au. In some specific embodiments, the metal M can be iridium (Ir), while the metal M can be platinum (Pt) in other specific embodiments. In some embodiments, R_4, R_5 or both can include metal M, while R_4 or R_5 can include metal M in other embodiments.

In some embodiments, at least one of R_1, R_2, and R_3 is aryl or substituted aryl. In some embodiments at least one of R_1, R_2, and R_3 is phenyl or substituted phenyl. In some embodiments, at least two of R_1, R_2, and R_3 are phenyl or substituted phenyl.

In some embodiments, each of R_1, R_2, and R_3 are either benzene or comprise metal M. In some embodiments, one of, or at least one of, R_1, R_2, and R_3 comprise metal M. In some embodiments, where R_1, R_2 or R_3 comprise metal M, the applicable R_1, R_2, or R_3 comprises aryl or substituted aryl comprising metal M.

In some embodiments, the compound is homoleptic, while the compound is heteroleptic in other embodiments. In embodiments where the compound is heteroleptic, another

ligand or part of the another ligand if the ligand is more than bidentate can be selected from the group consisting of:



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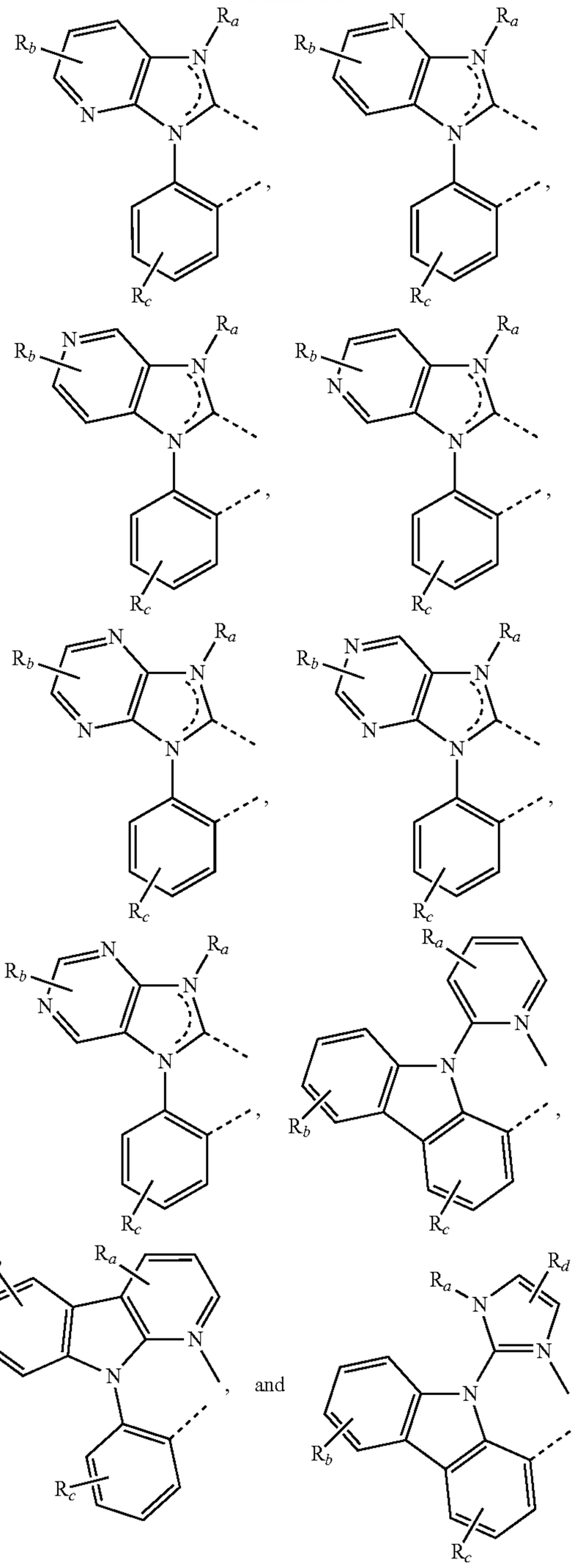


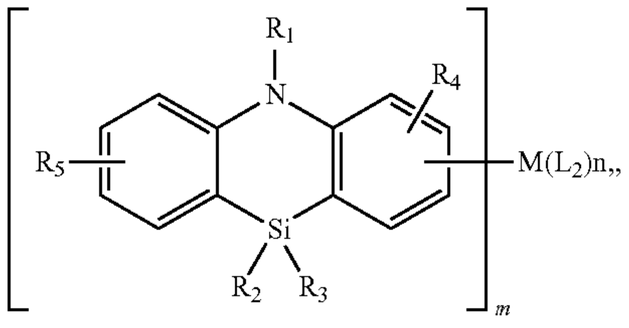
wherein R_a, R_b, R_c, and R_d may represent mono, di, tri, or tetra substitution, or no substitution;

wherein R_a, R_b, R_c, and R_d are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein two adjacent substituents of R_a, R_b, R_c, and R_d are optionally joined to form a fused ring or form a multidentate ligand.

In some embodiments, the compound can have the formula:

Formula II



wherein L_2 is another ligand coordinated to the metal M;

wherein each L_2 can be same or different;

wherein m is a value from 1 to the maximum number of ligands that may be attached to the metal M;

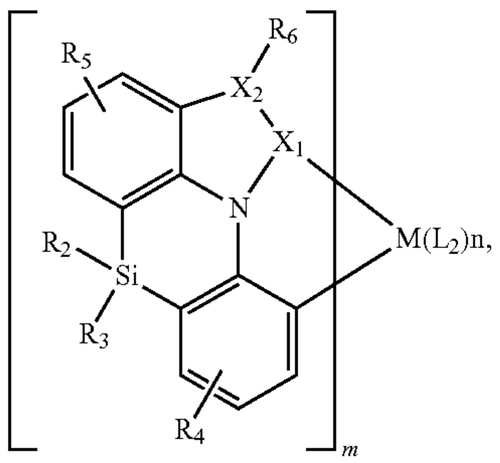
wherein m+n is the maximum number of ligands that may be attached to the metal M; and

wherein any of R_1, R_2, R_3, and R_4 are optionally linked to L_2 to comprise a bidentate, tridentate, tetradentate, pentadentate or hexadentate ligand.

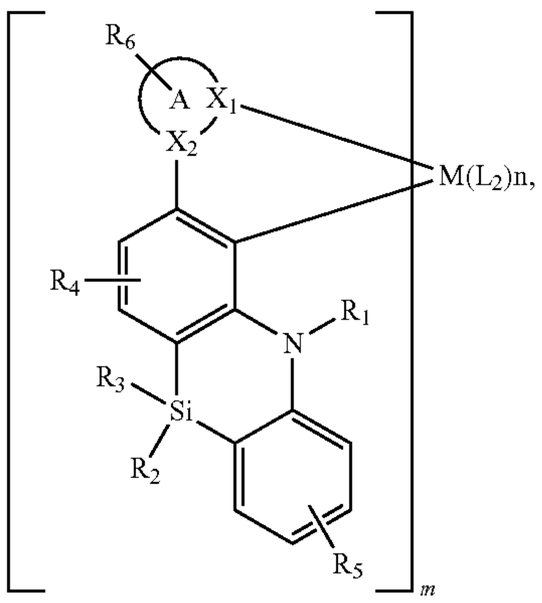
In some compounds of Formula II, at least one of R_1, R_2, R_3, and R_4 are linked to L_2 to comprise a bidentate, tridentate, tetradentate, pentadentate or hexadentate ligand.

In some more compounds of Formula II, the compound can be selected from the group consisting of:

GS 1



GS 2



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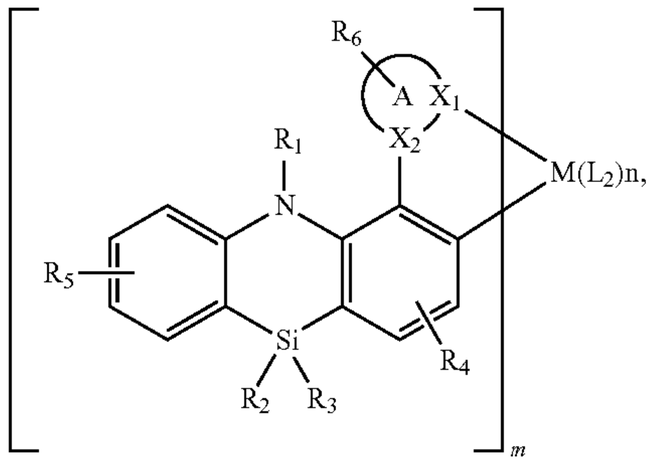
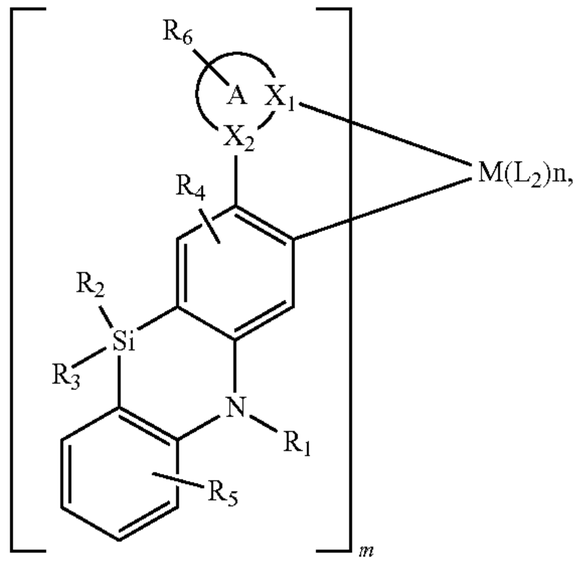
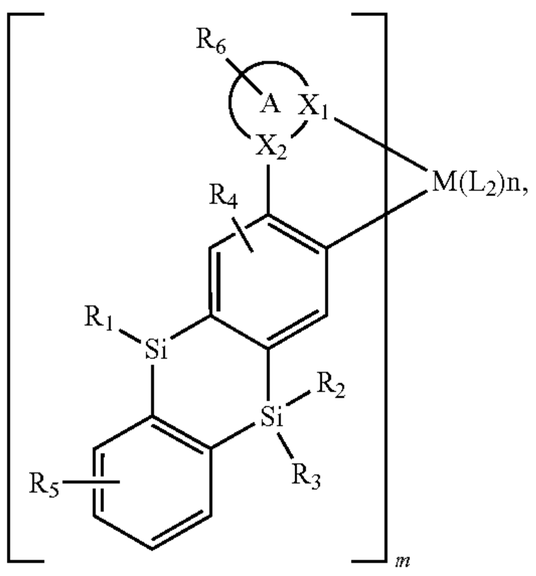
GS 3



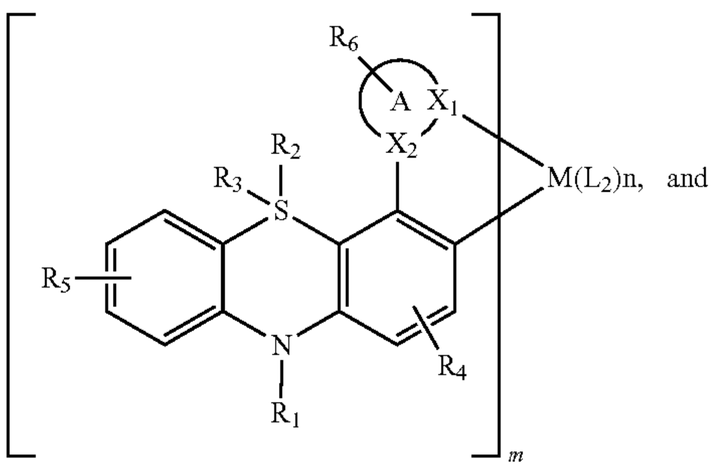
GS 4



GS 5



GS 6



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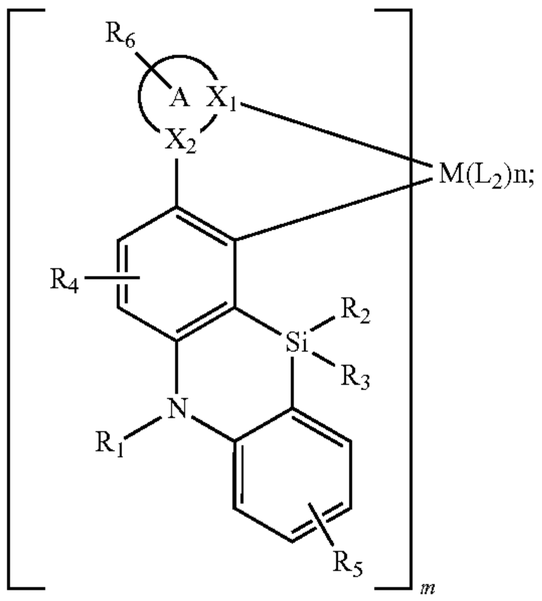


wherein X_1, X_2 is selected from the group consisting of C, N, O, P, S, and B;

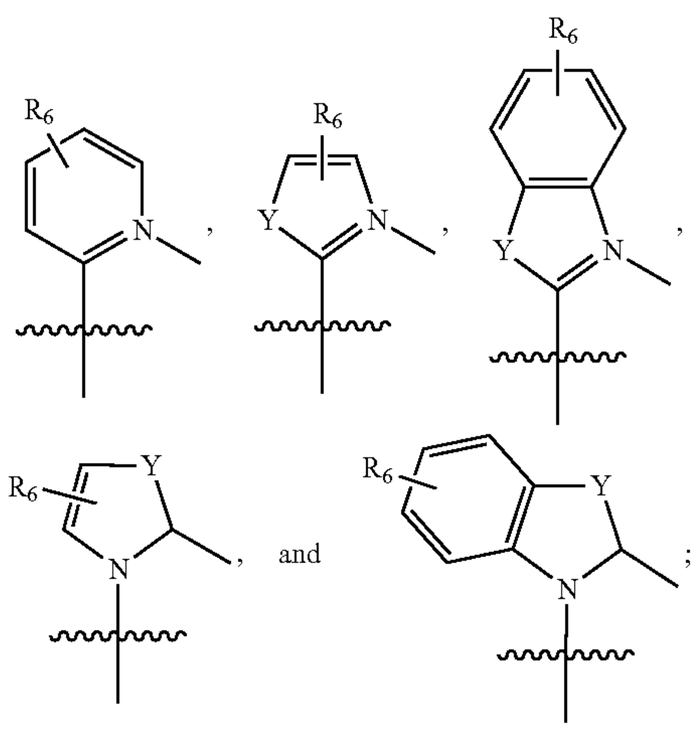
wherein A is a 5-membered or 6-membered carbocyclic or heterocyclic ring;

wherein R_6 represents mono, di, tri, tetra substitutions or no substitution;

wherein R_6 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein any two adjacent R_1, R_2, R_3, R_4, R_5, and R_6 are optionally joined to form a ring, which may be further substituted.

In some of the embodiments of Formula II, A can be selected from the group consisting of:



wherein Y is selected from the group consisting of BR, NR, PR, O, S, Se, C═O, S═O, SO_2, CRR', SiRR', and GeRR';

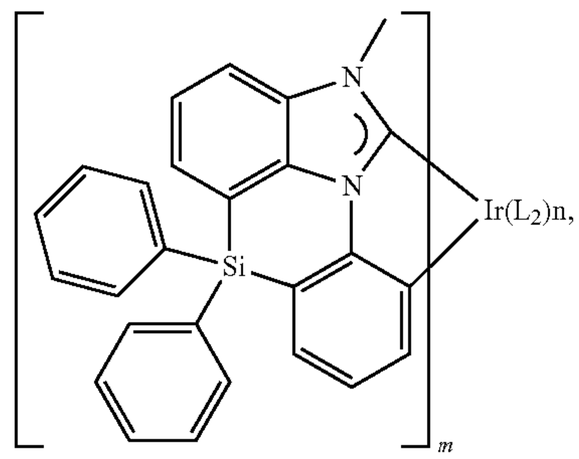
wherein R, R' are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein R, R' are optionally joined to form a ring with any adjacent substituent.

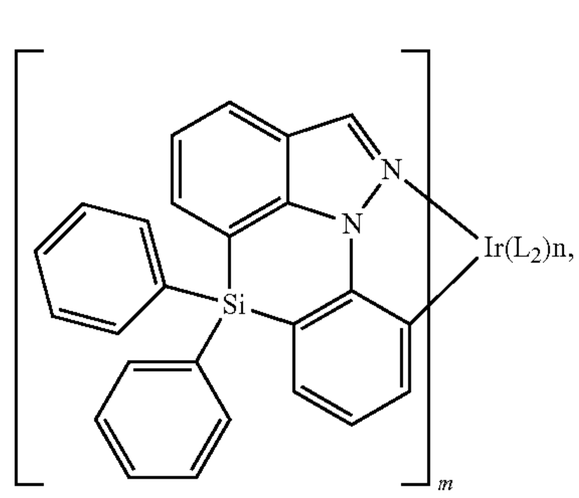
In some specific embodiments, the compound can be selected from the group consisting of:

GS 7

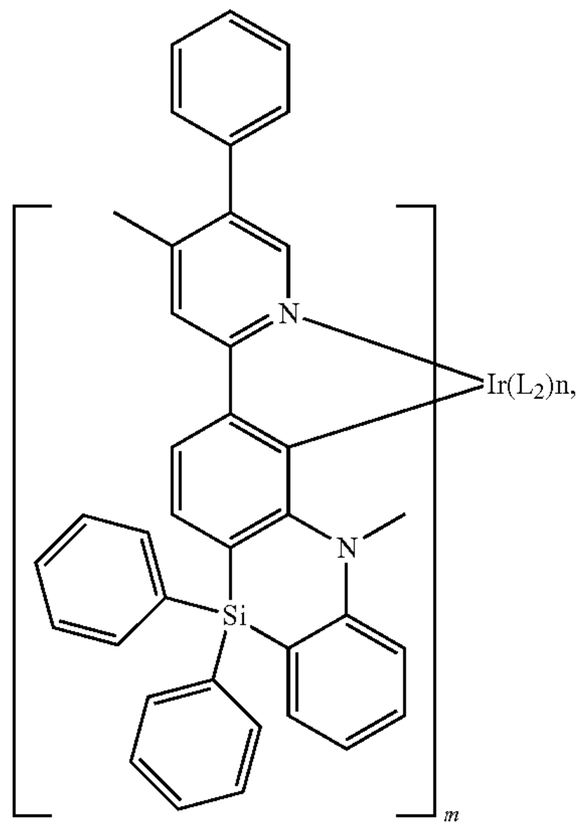
Compound 1-1



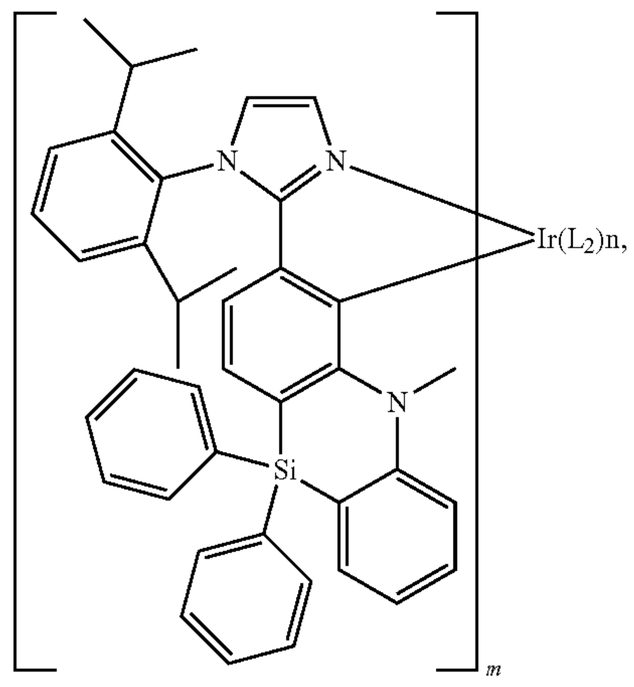
Compound 1-2



Compound 2-1



Compound 2-2



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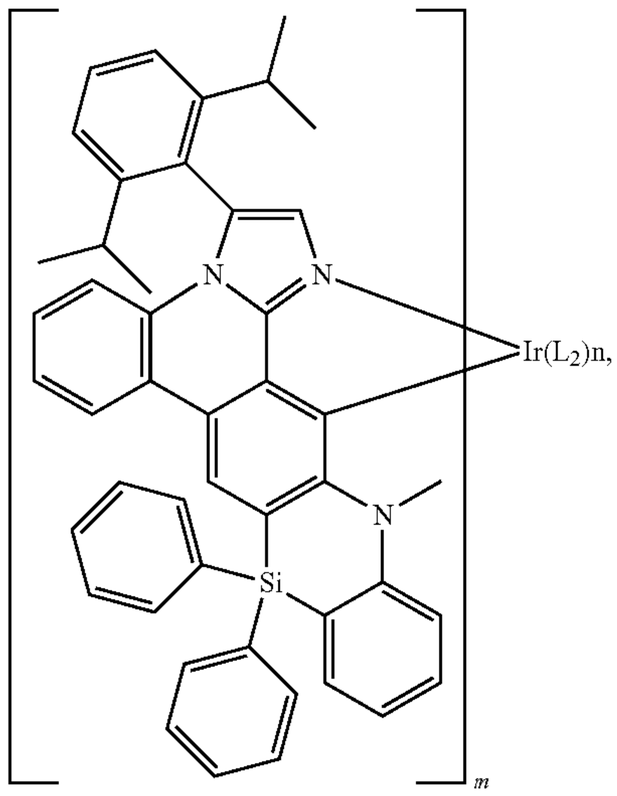
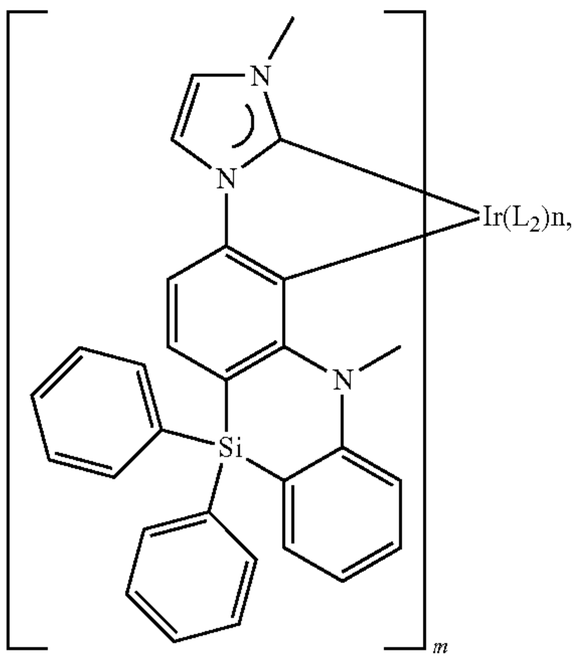
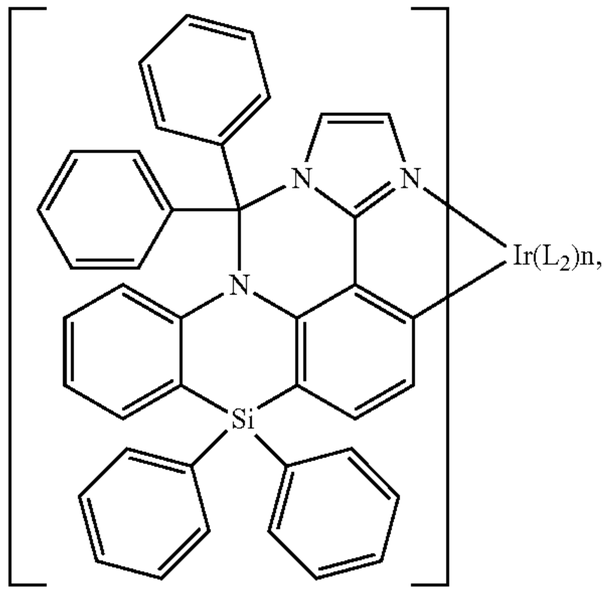
Compound 2-3



Compound 2-4



Compound 3-1



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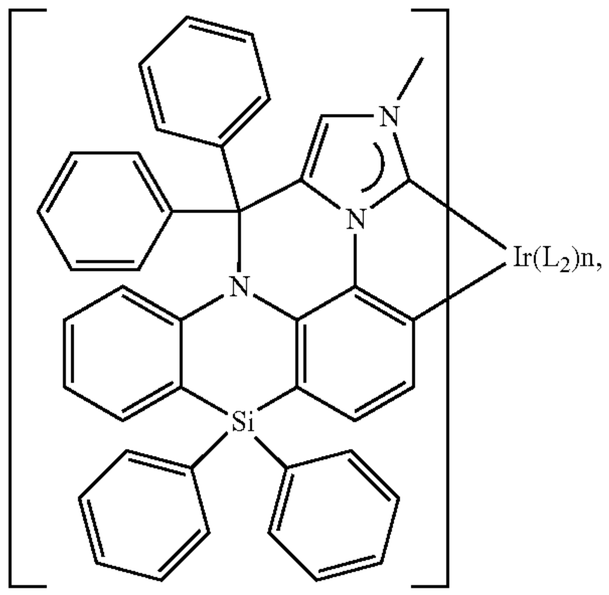
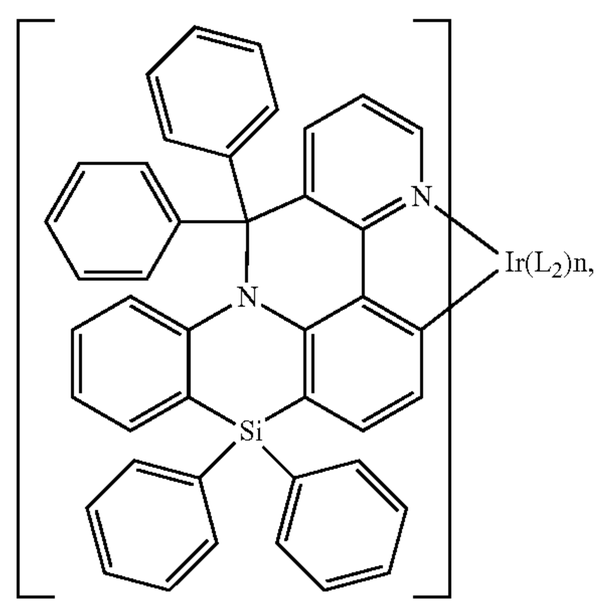
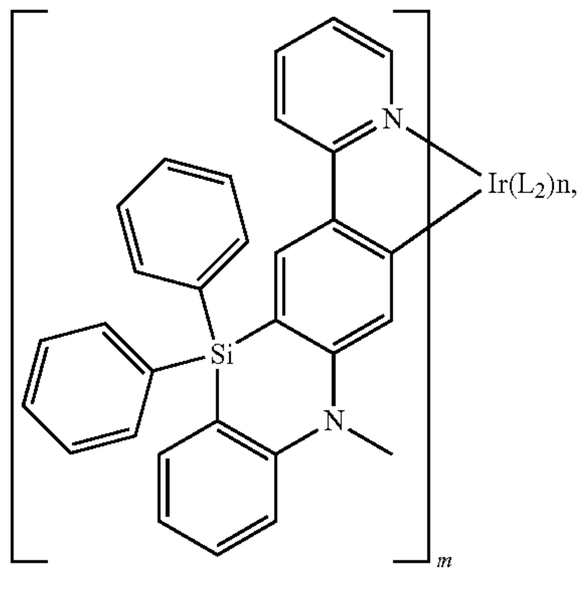
Compound 3-2



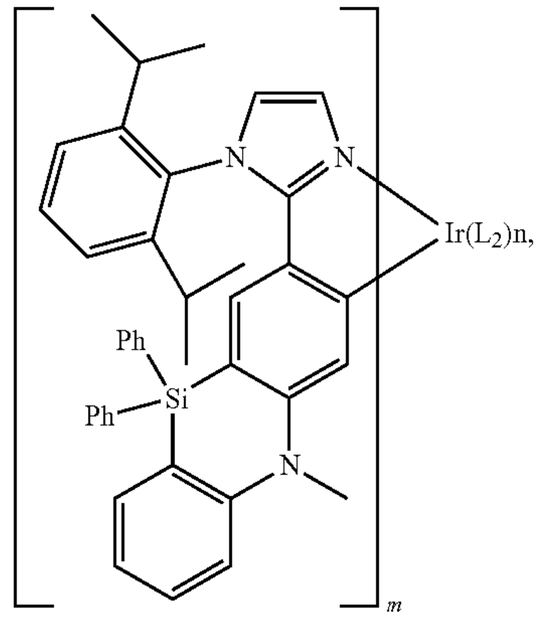
Compound 3-3



Compound 4-1



Compound 4-2



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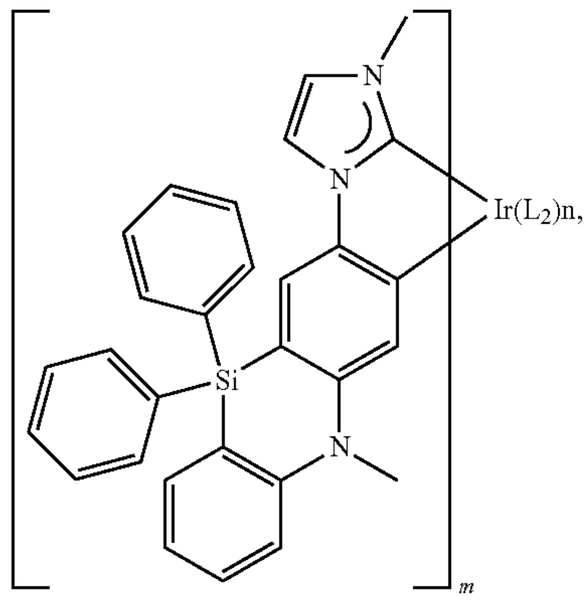
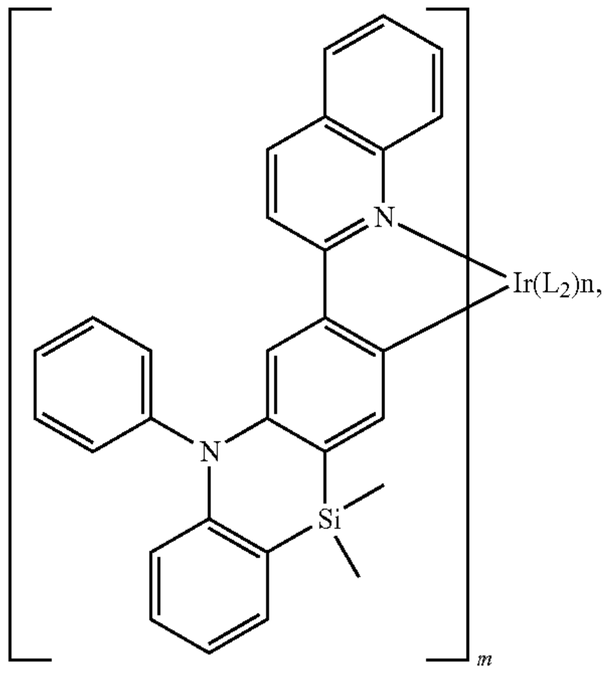
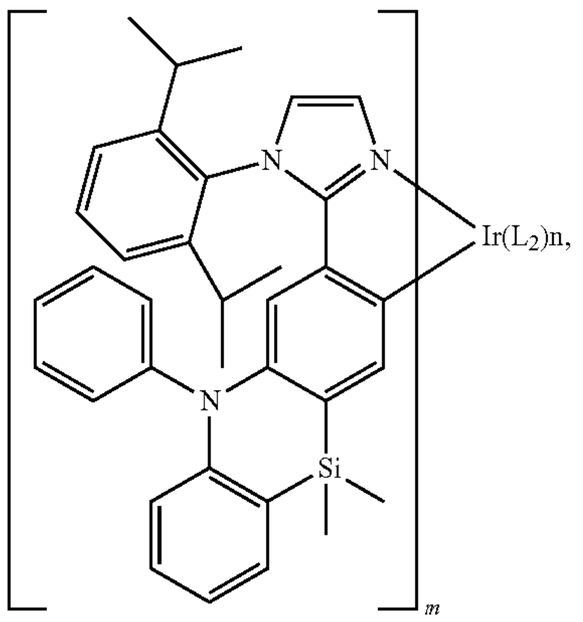
Compound 4-3



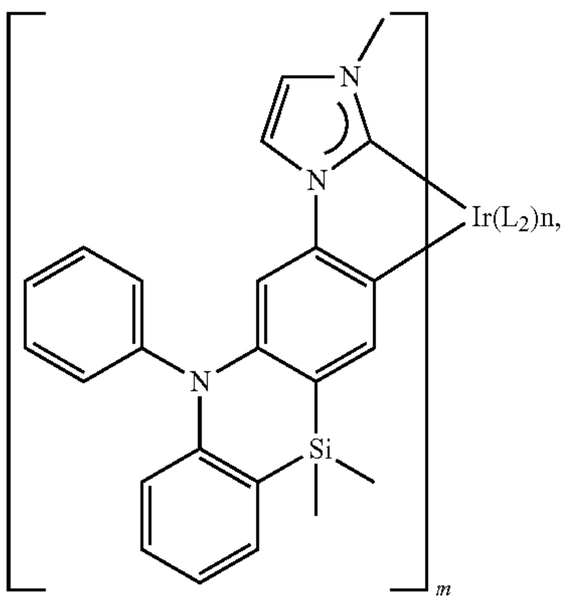
Compound 5-1



Compound 5-2



Compound 5-3



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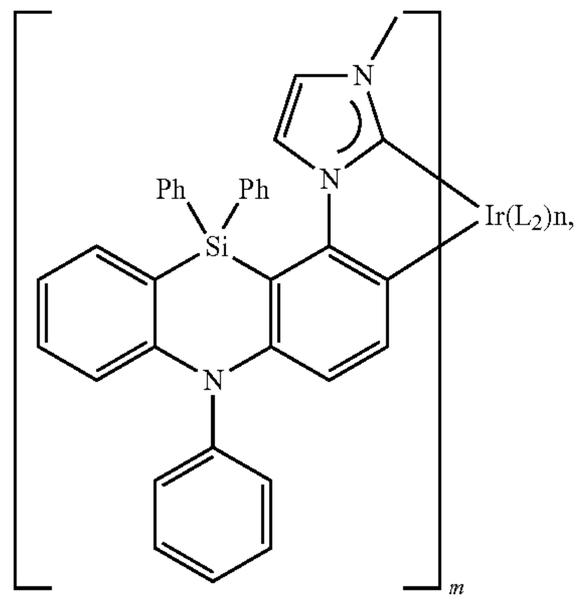
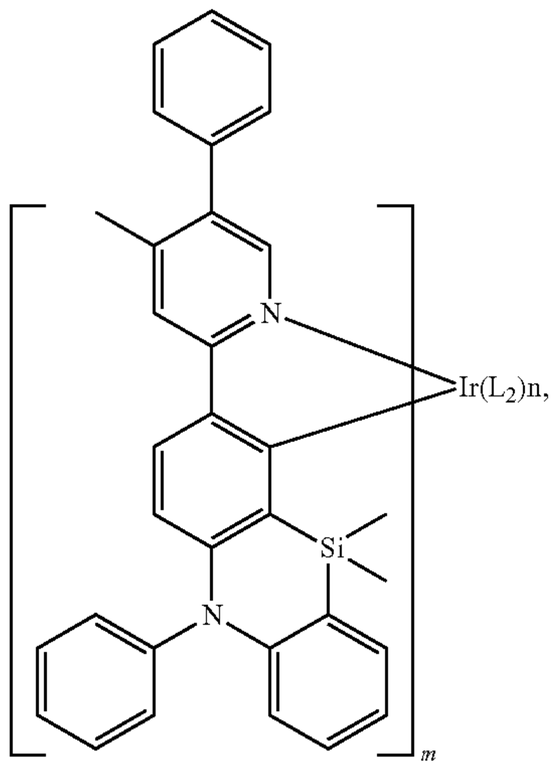
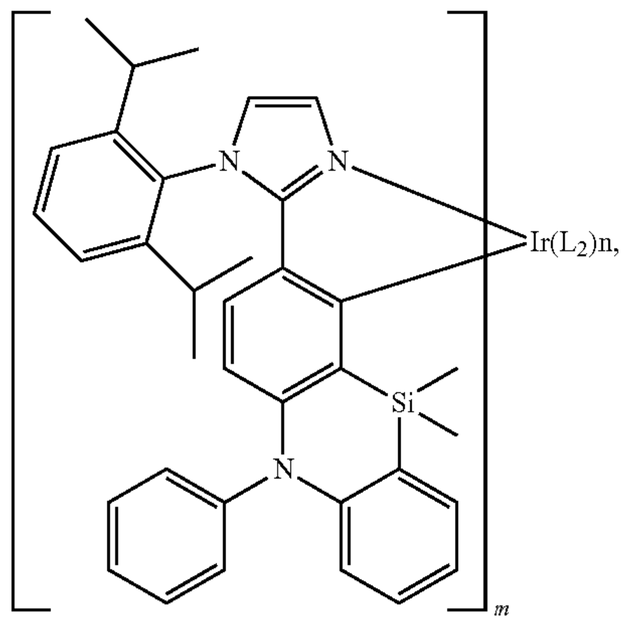
Compound 6-1



Compound 7-1



Compound 7-2



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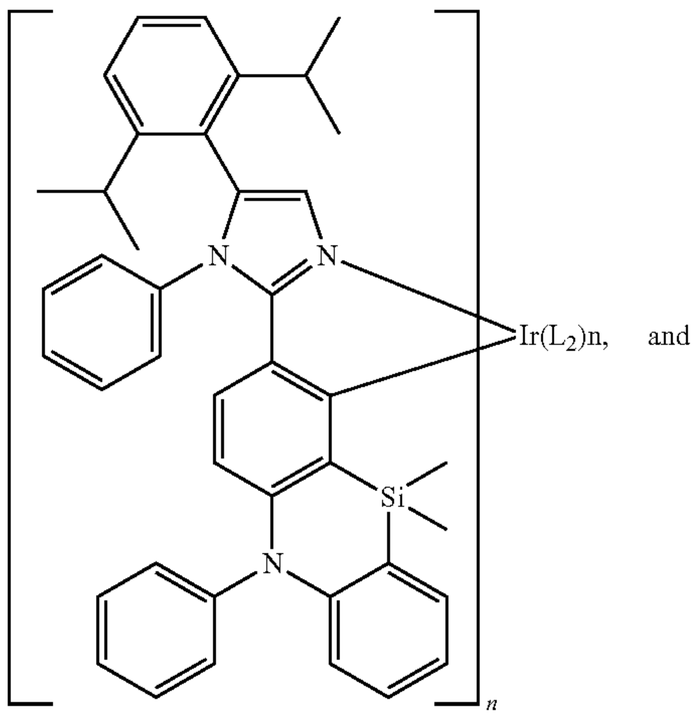
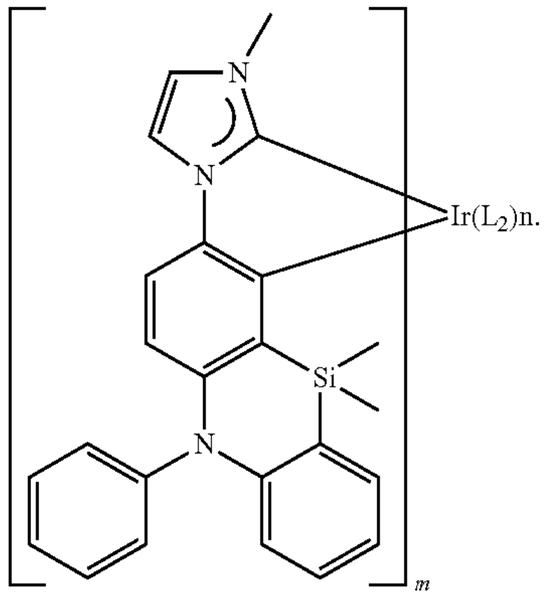
Compound 7-3



and

Compound 7-4



In some embodiments of Formula II, m is 3, and n is 0. In other embodiments, m is 1, and n is 2. In some more specific embodiments, L_2 is selected from the group consisting of:

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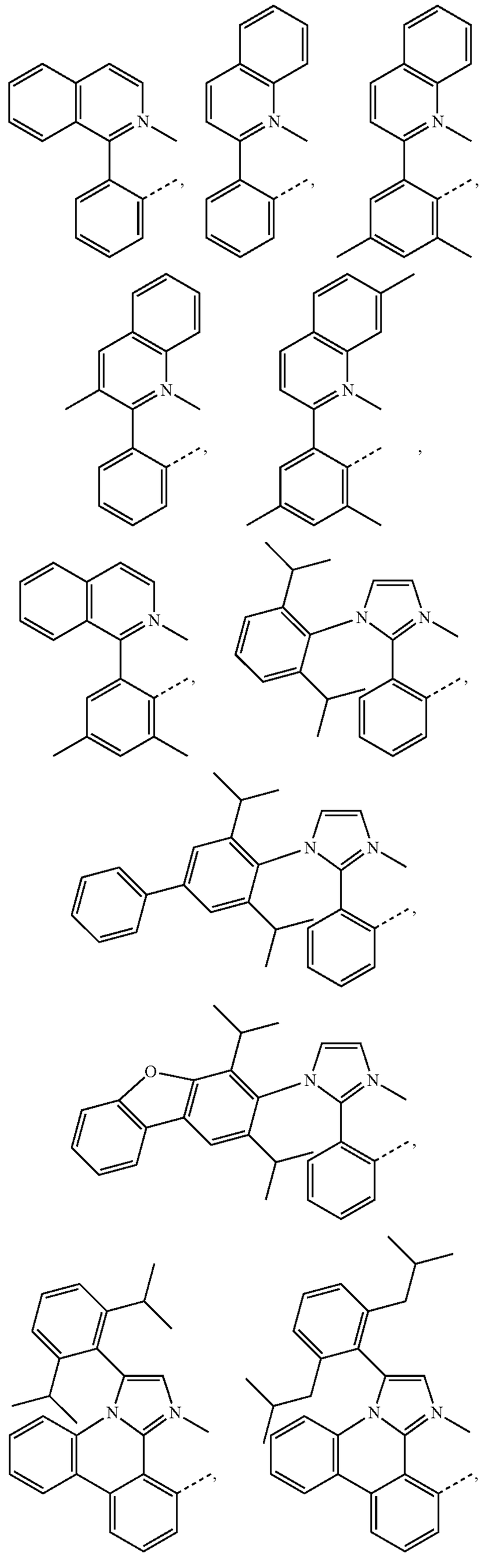

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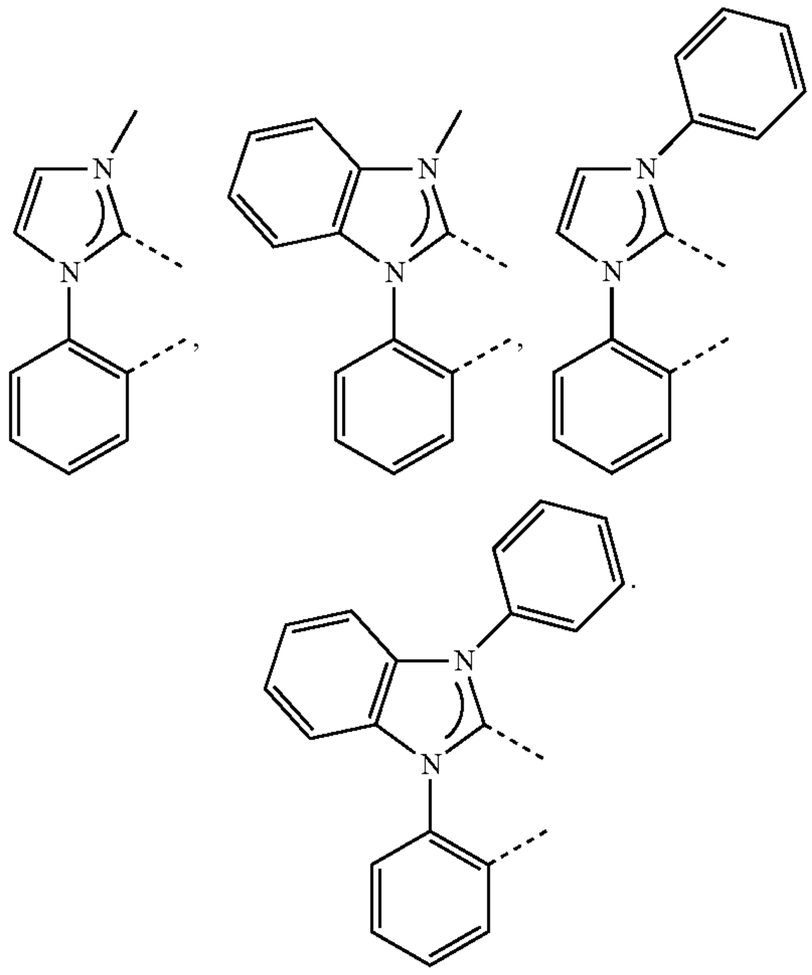

, and

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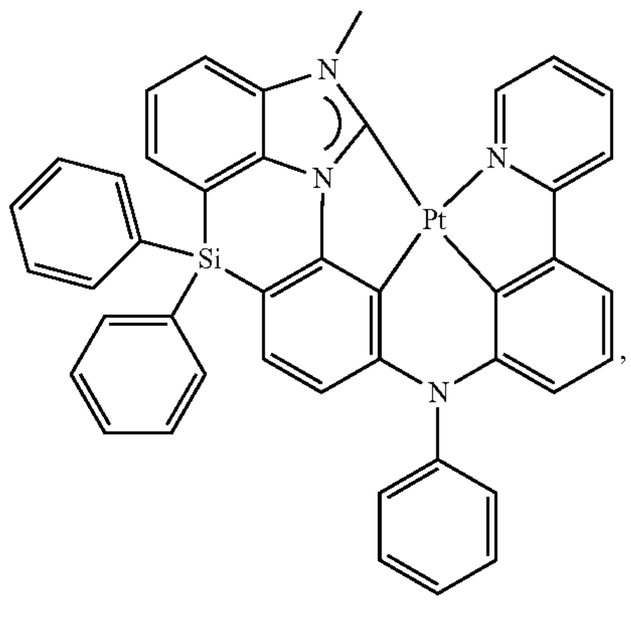
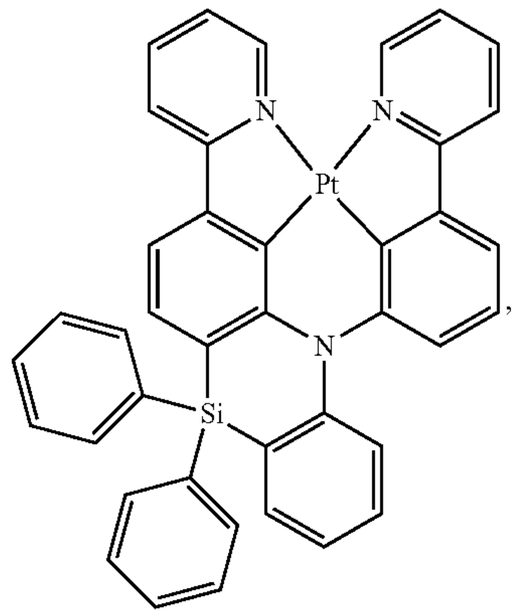
Compound 1-14

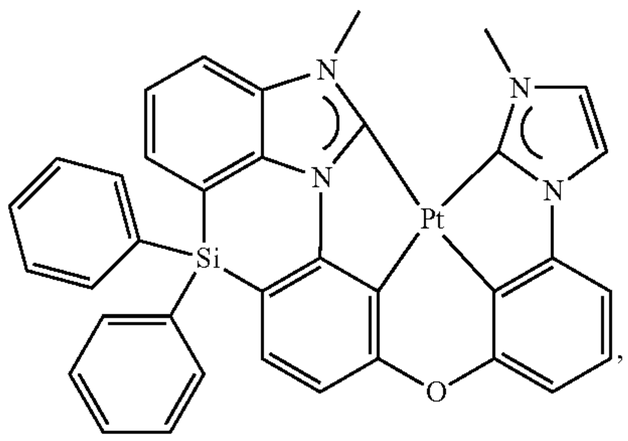


Compound 2-11

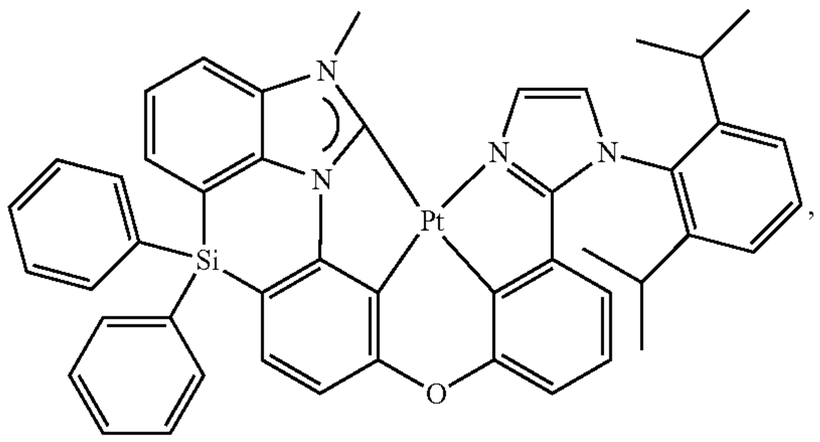


In some specific embodiments, the compound is selected from the group consisting of:

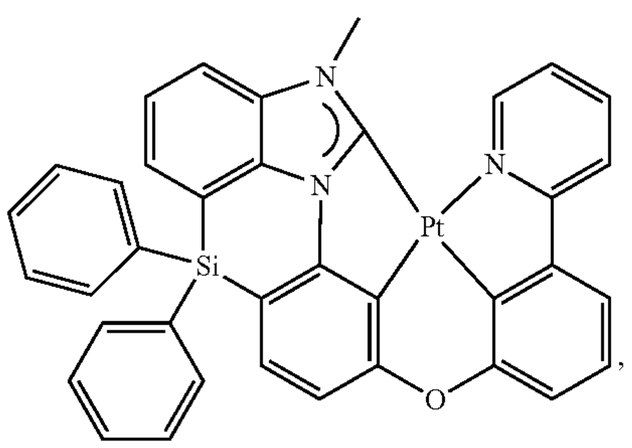
Compound 1-11



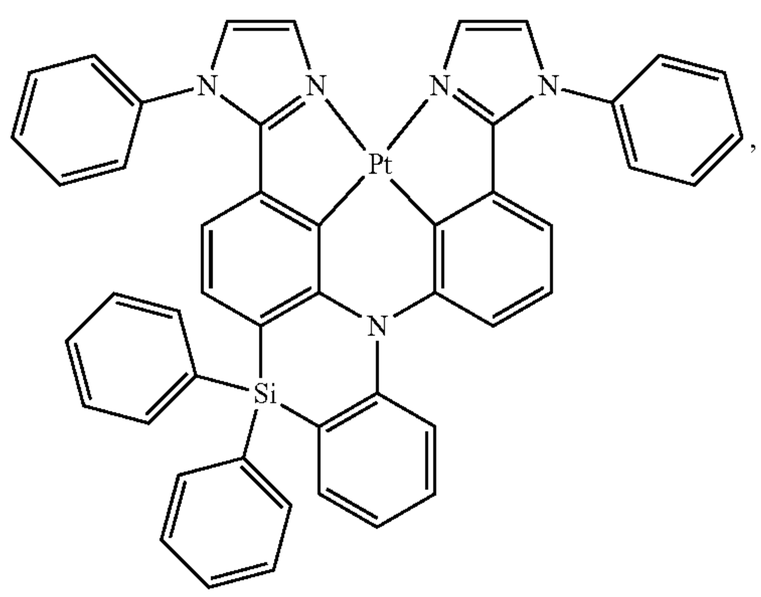
Compound 1-12



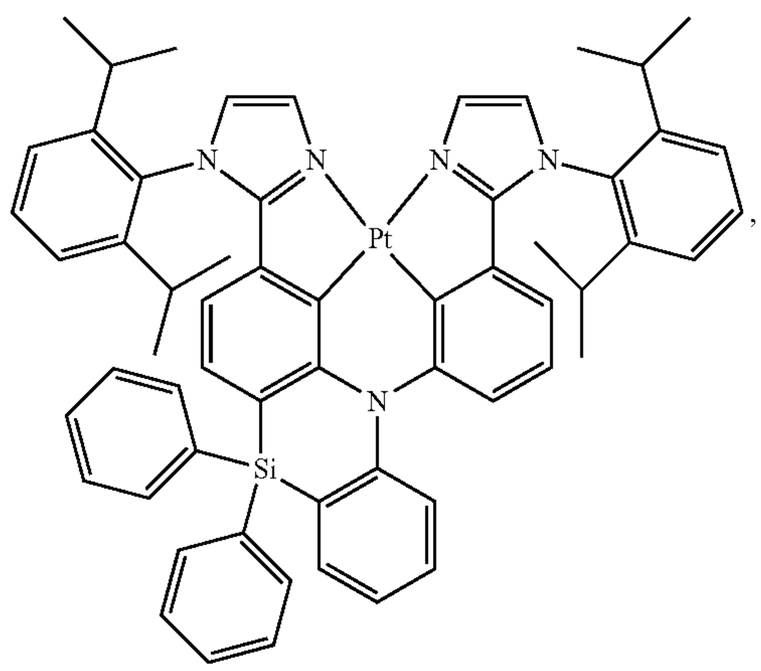
Compound 1-13



Compound 2-12



Compound 2-13



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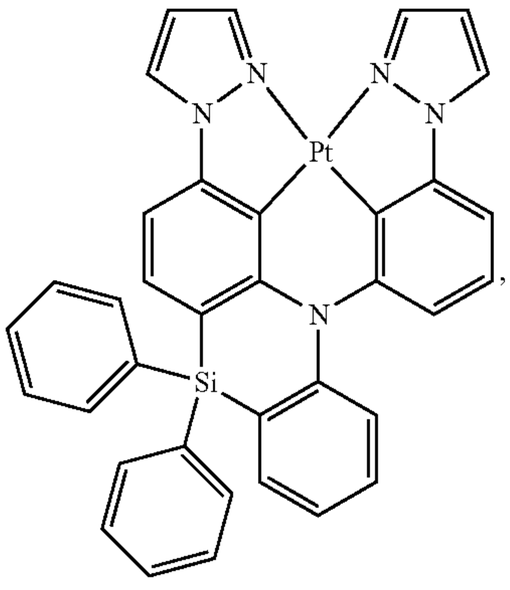
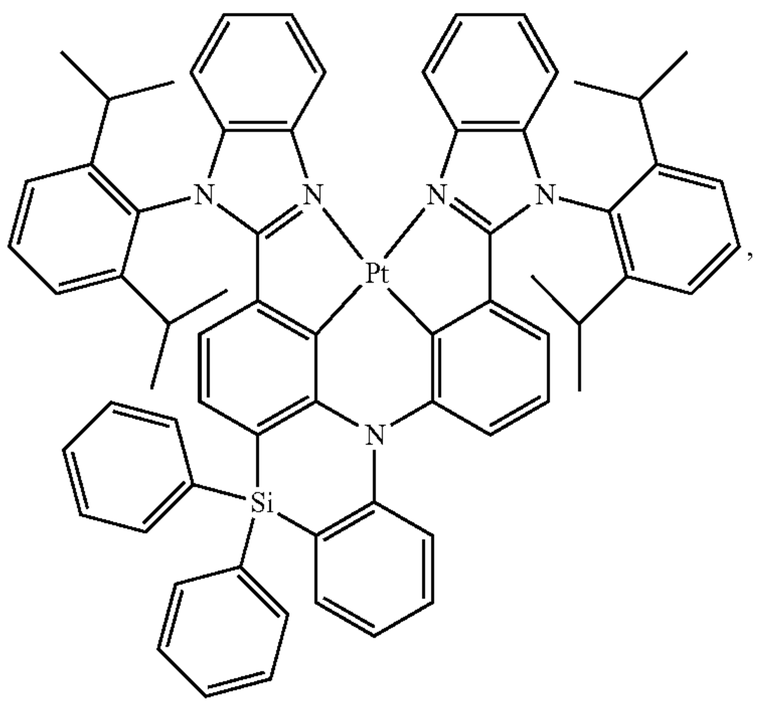
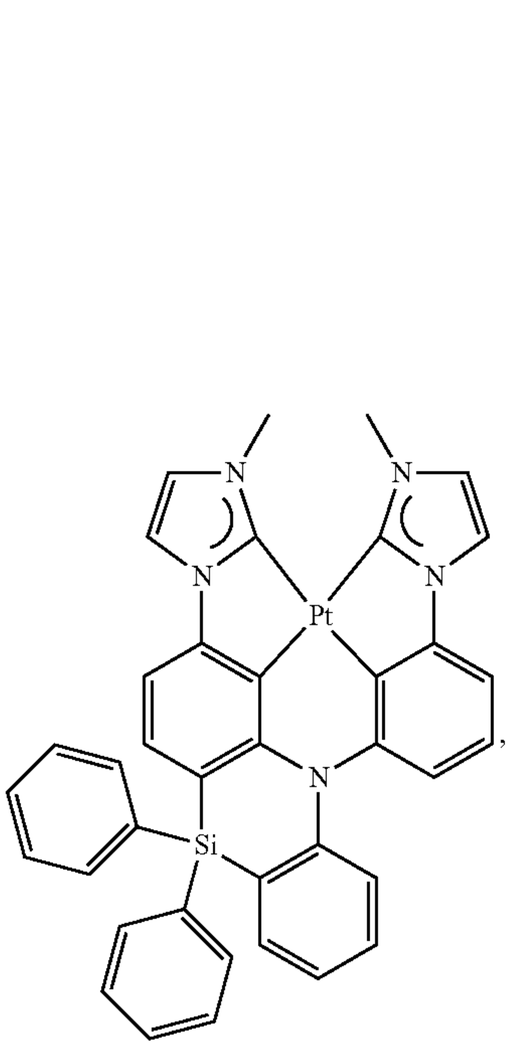
Compound 2-14



Compound 2-15



Compound 2-16



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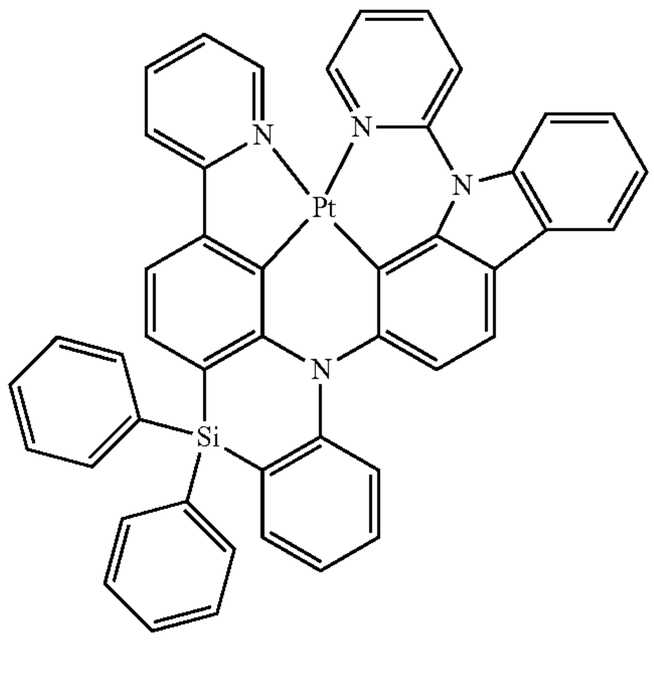
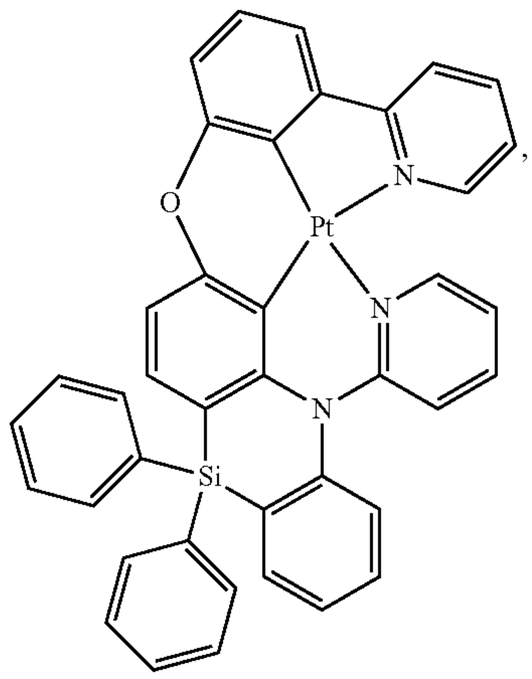
Compound 2-17



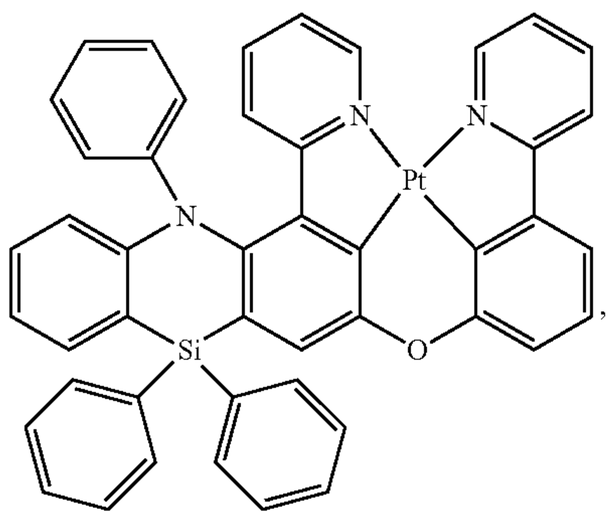
Compound 2-18



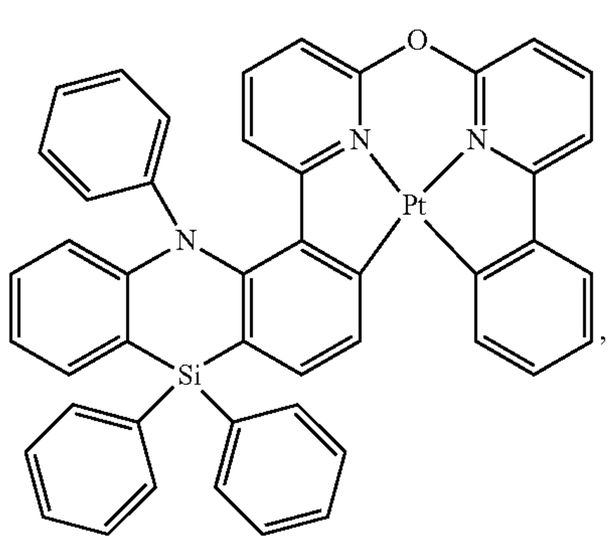
Compound 2-19

-continued

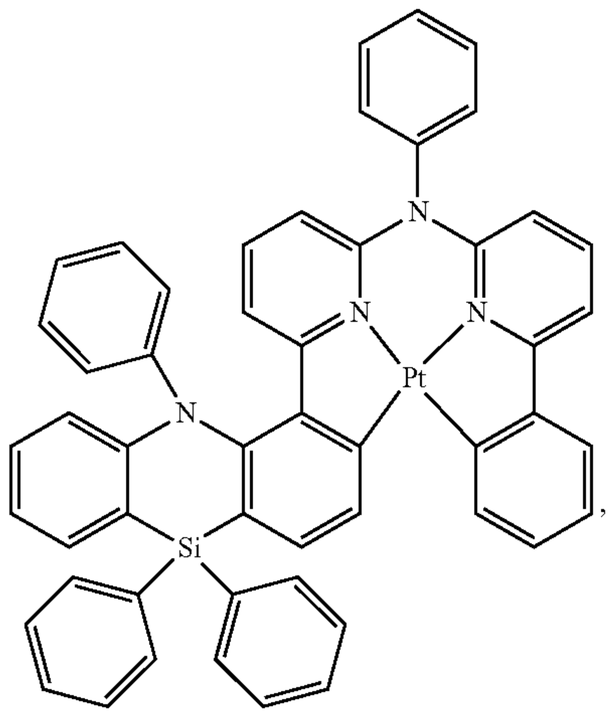
Compound 3-11



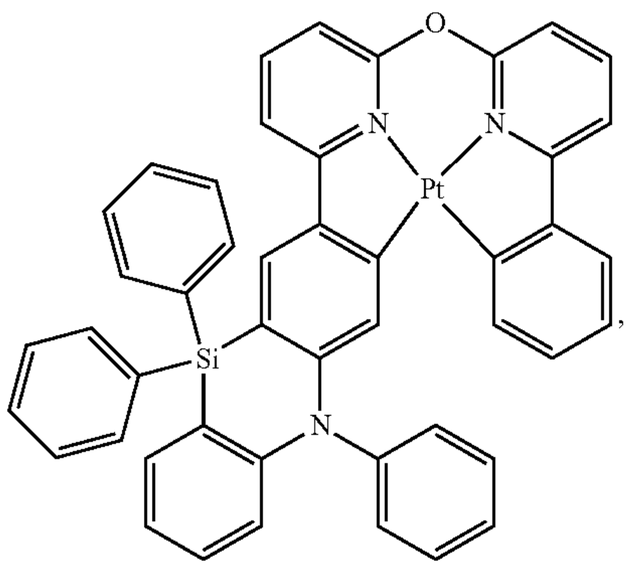
Compound 3-12



Compound 3-13



Compound 4-11



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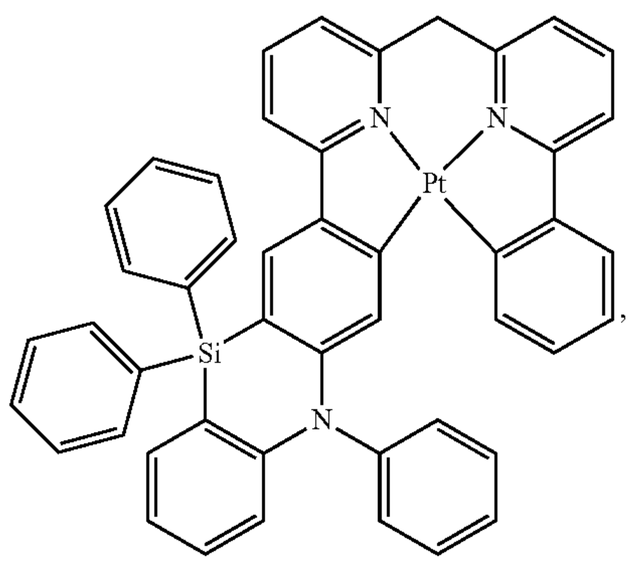
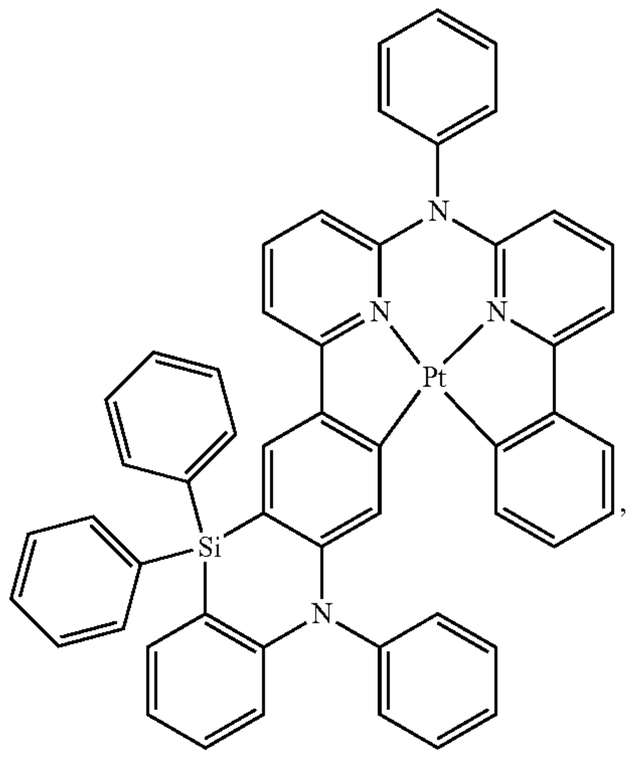
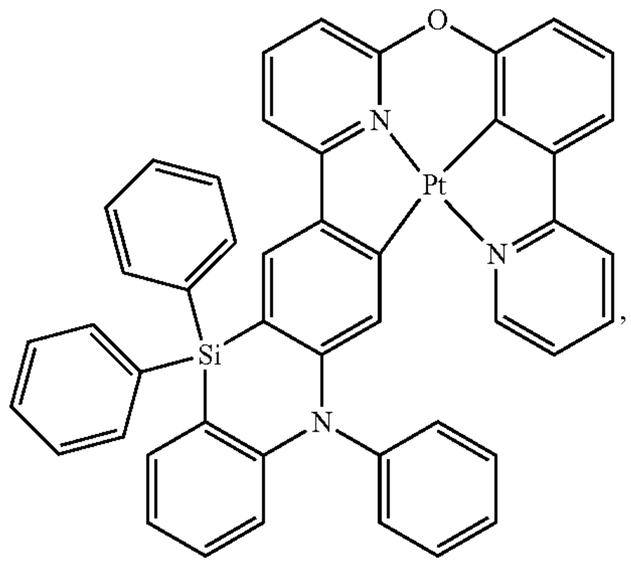
Compound 4-12



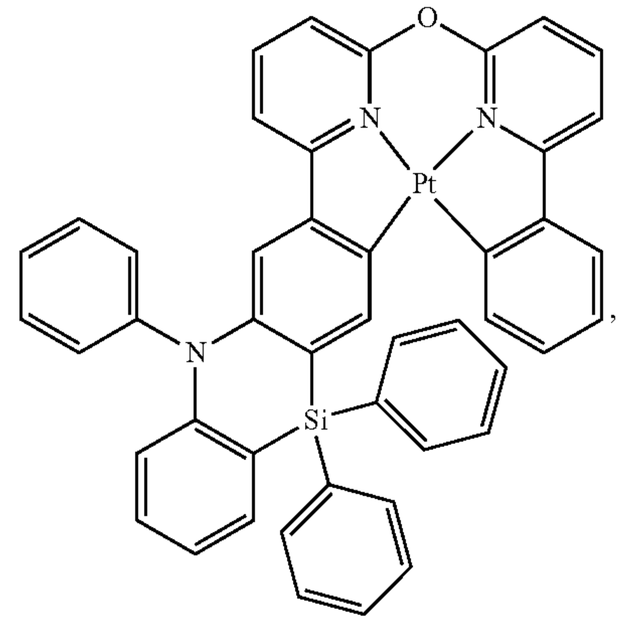
Compound 4-13



Compound 4-14



Compound 5-11



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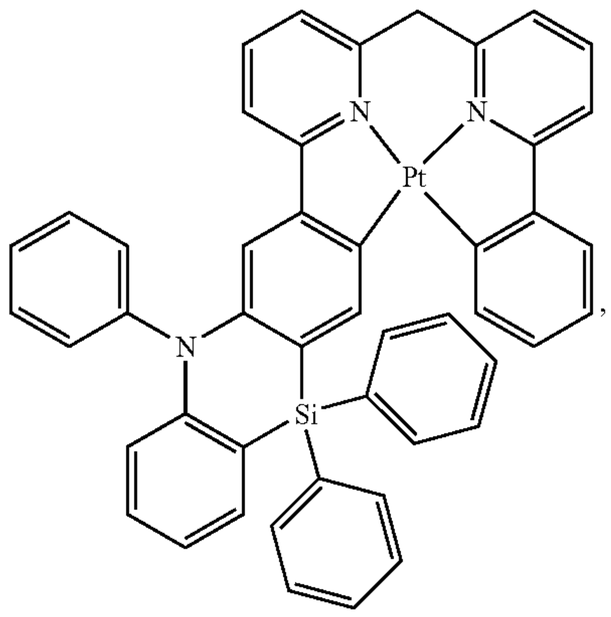
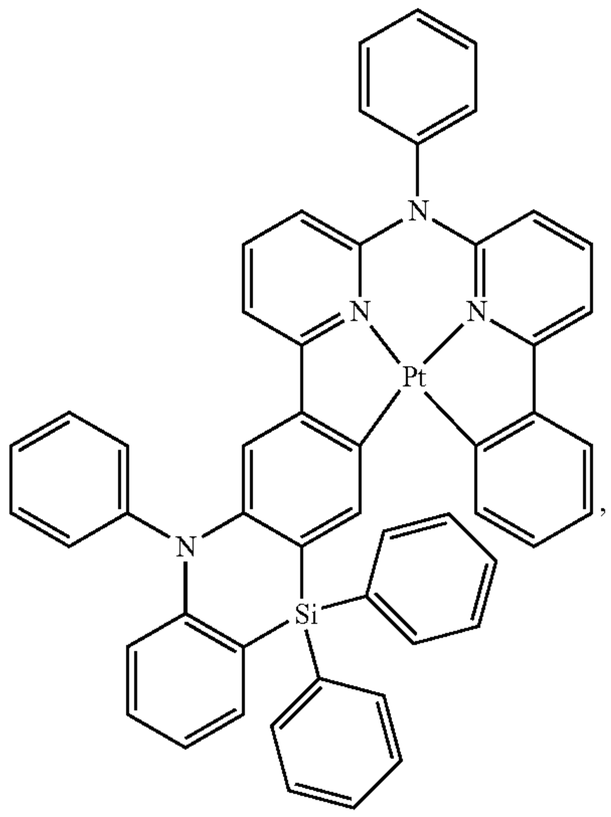
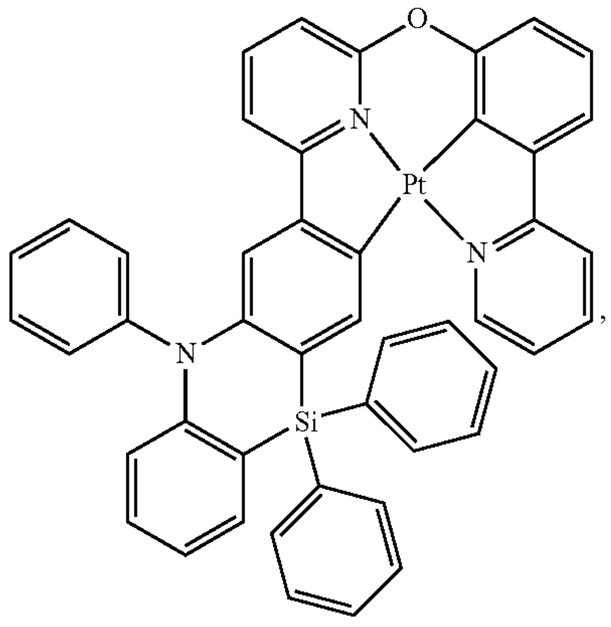
Compound 5-12



Compound 5-13



Compound 5-14



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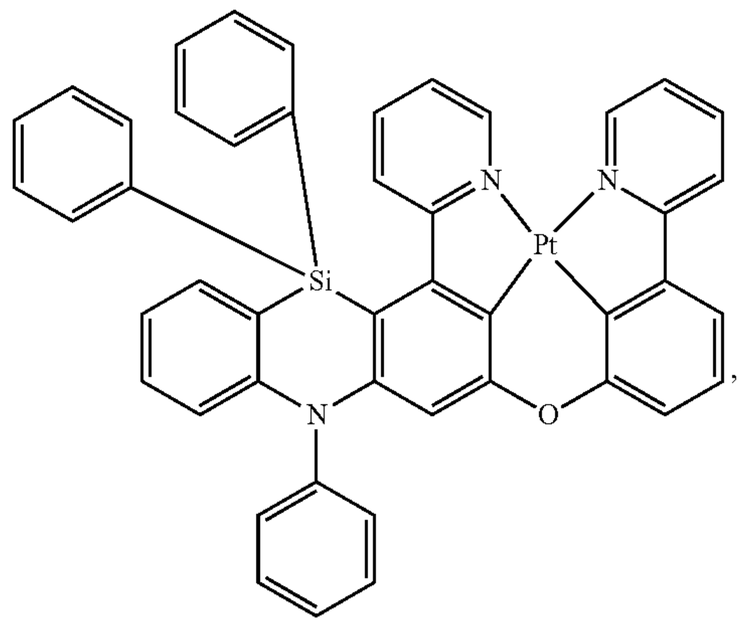
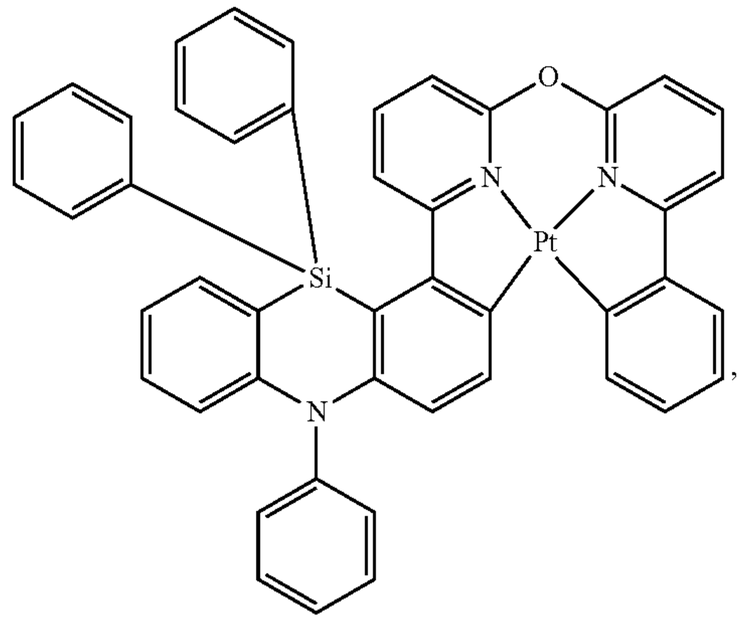
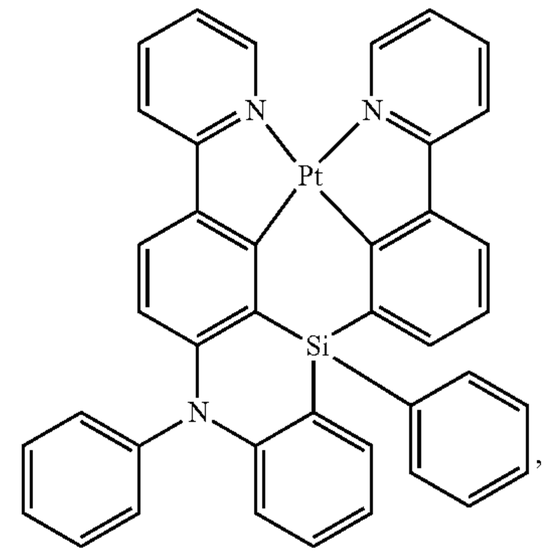
Compound 6-11



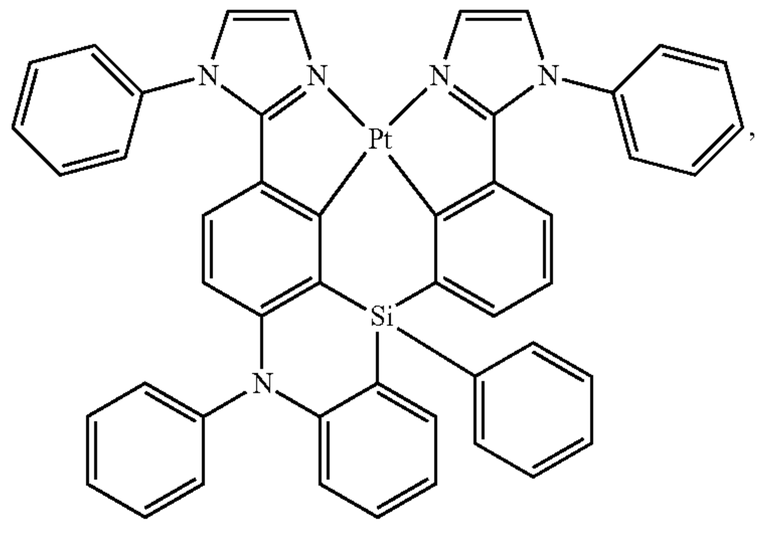
Compound 6-12



Compound 7-11



Compound 7-12



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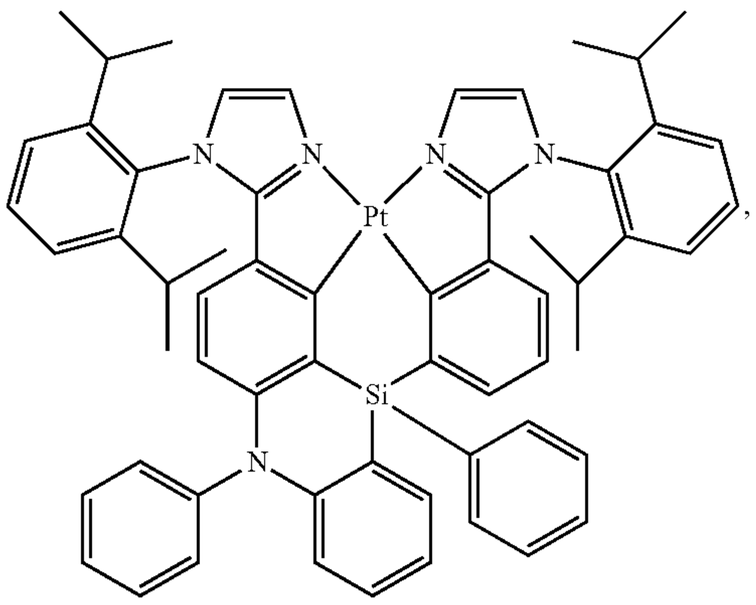
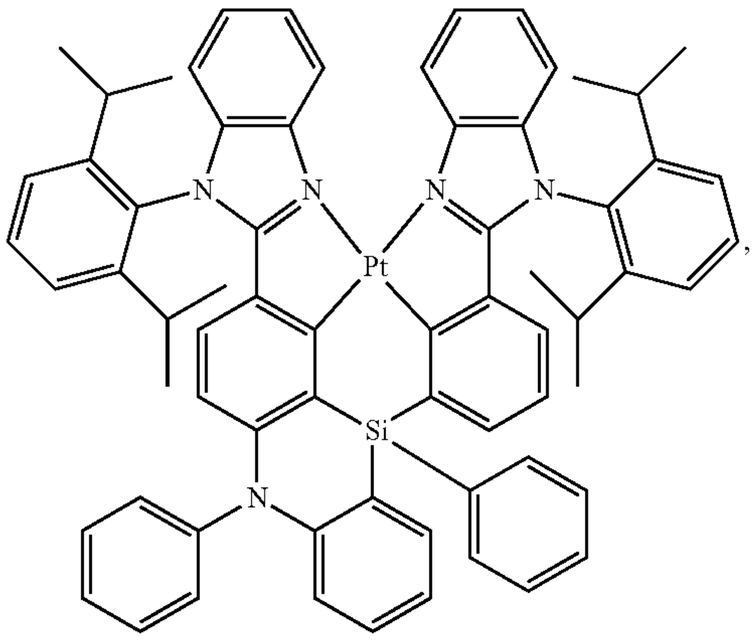
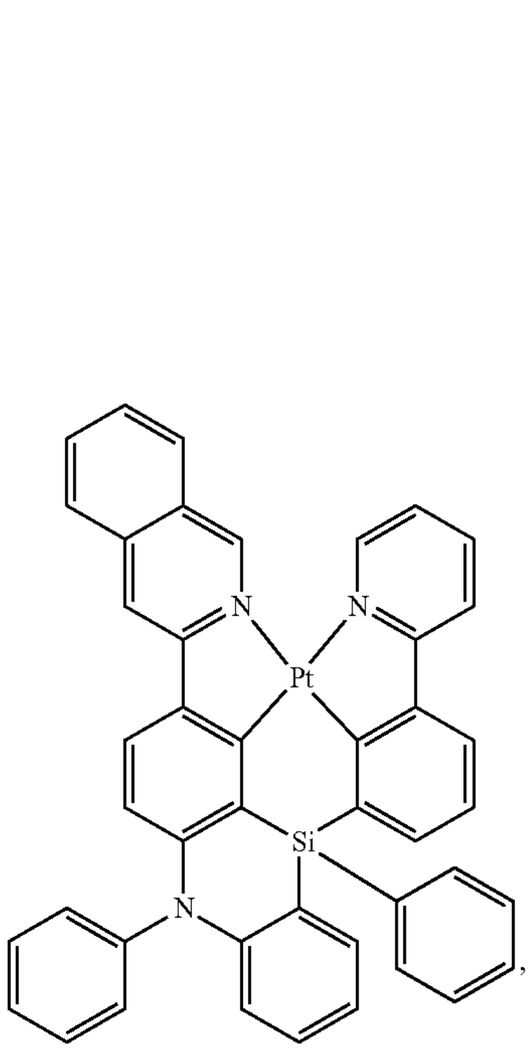
Compound 7-13



Compound 7-14



Compound 7-15



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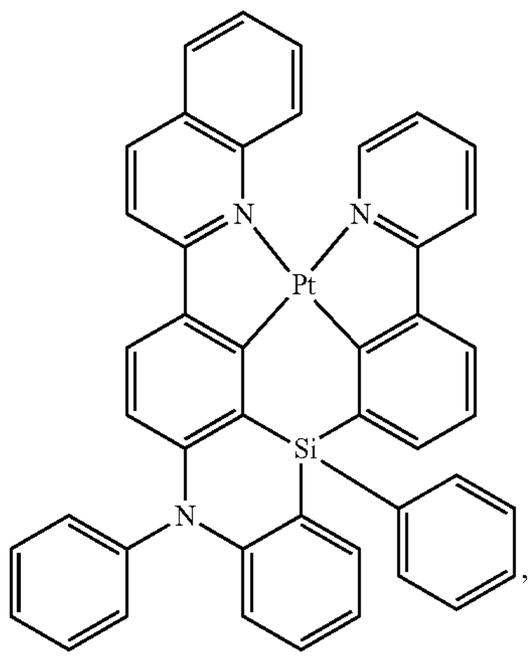
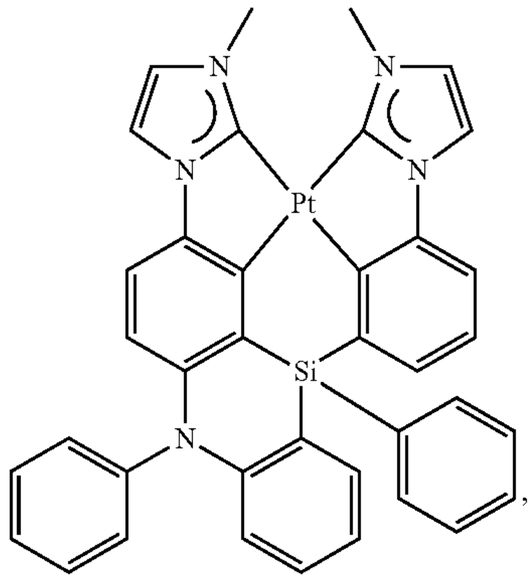
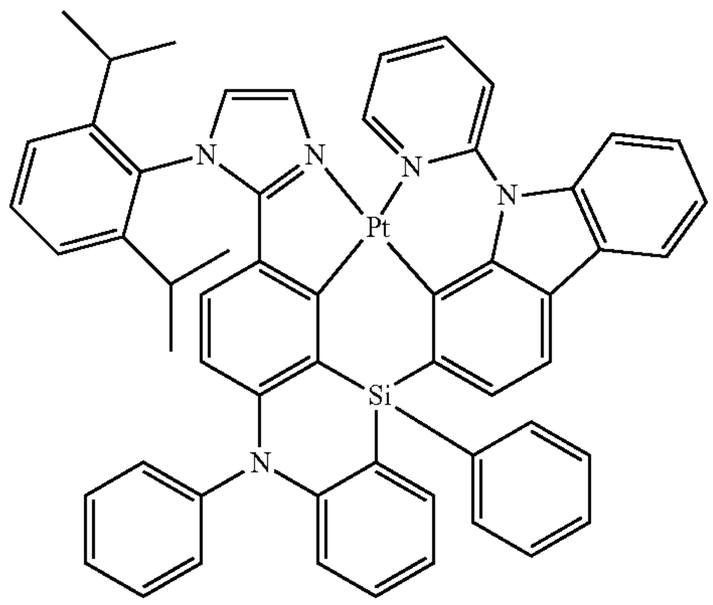
Compound 7-16



Compound 7-17

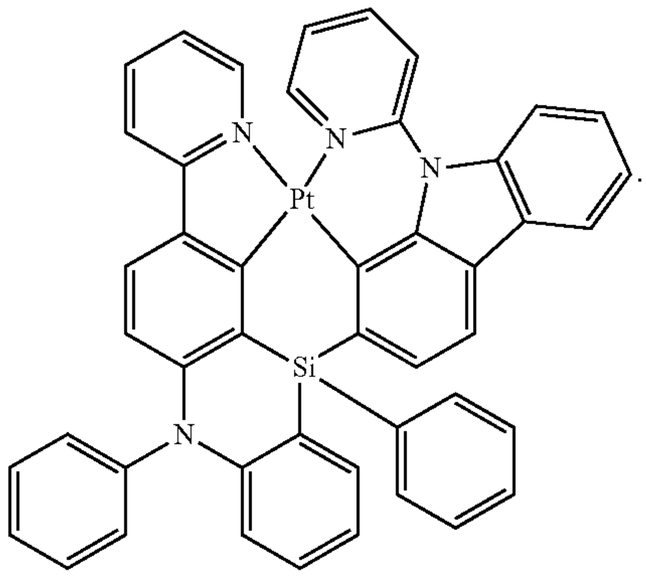


Compound 7-18



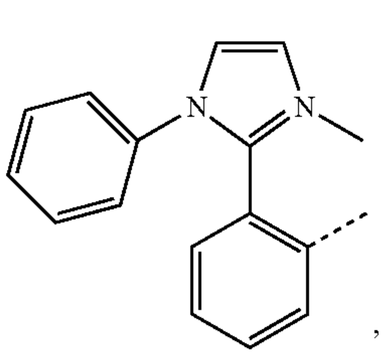
and

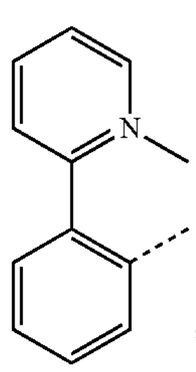
Compound 7-19



In some embodiments, R_1 includes a 5-membered or 6-membered carbocyclic or heterocyclic aromatic ring; and

R_1 is coordinated to the metal M. In some embodiments, R_2 includes a 5-membered or 6-membered carbocyclic or heterocyclic aromatic ring; and R_2 is coordinated to the metal M. In some embodiments, R_1, or R_2, or both, include at least one of the chemical groups selected from the group consisting of:


,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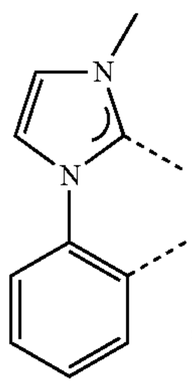
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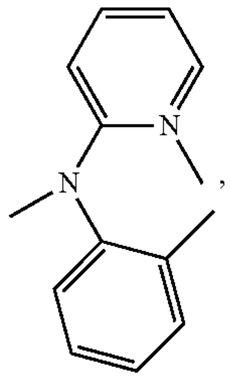
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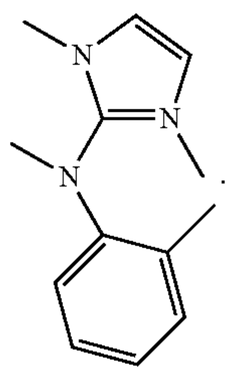
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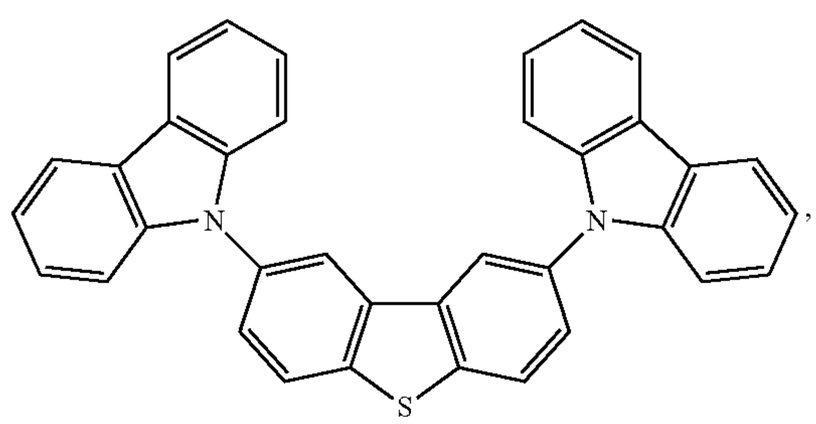
According to another aspect of the present disclosure, a first device is also provided. The first device includes a first organic light emitting device, that includes an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer can include a compound including L_1 coordinated to a metal M as described herein, and variations thereof. In some embodiments, the organic layer can include a compound of Formula II as described herein, and variations thereof.

The first device can be one or more of a consumer product, an organic light-emitting device and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

The organic layer can also include a host. In some embodiments, the host can include a metal complex. The host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, OC_nH_{2n+1}, OAr_1, $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH{=}CH{-}C_nH_{2n+1}$, $C{\equiv}C{-}C_nH_{2n+1}$, Ar_1, $Ar_1{-}Ar_2$, $C_nH_{2n}{-}Ar_1$, or no substitution. In the preceding substituents n can range from 1 to 10; and Ar_1 and Ar_2 can be independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

The host can be a compound selected from the group consisting of carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. The "aza" designation in the fragments described above, i.e., aza-dibenzofuran, aza-dibenzonethiophene, etc., means that one or more of the C—H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline and dibenzo[f,h]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein. The host can include a metal complex. The host can be a specific compound selected from the group consisting of: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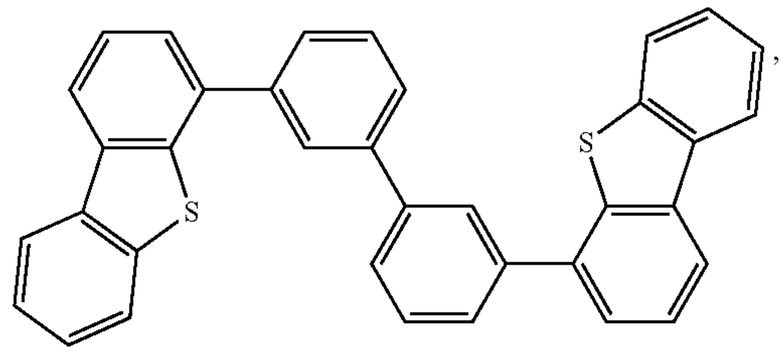
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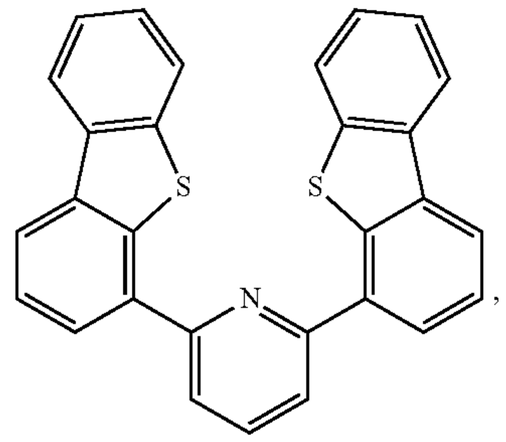
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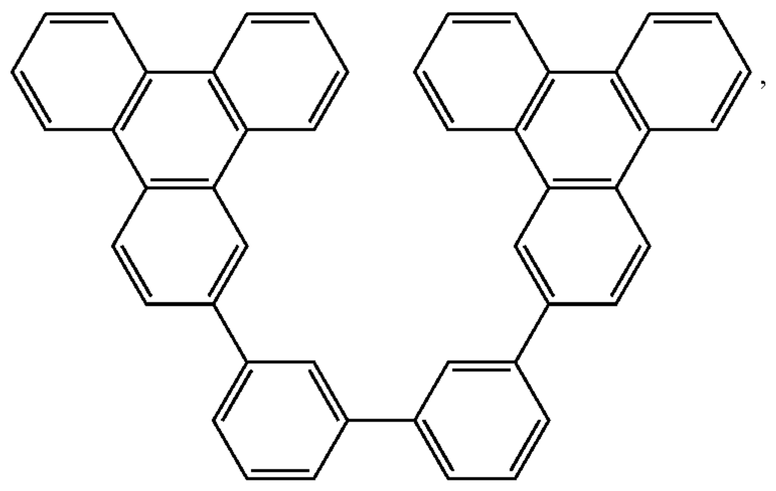
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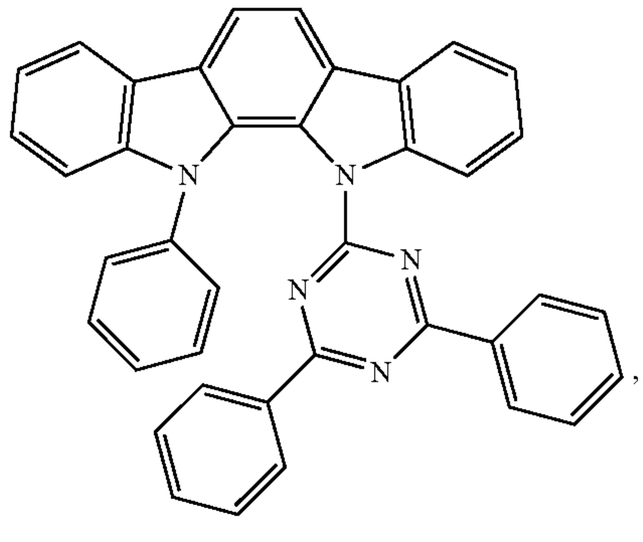
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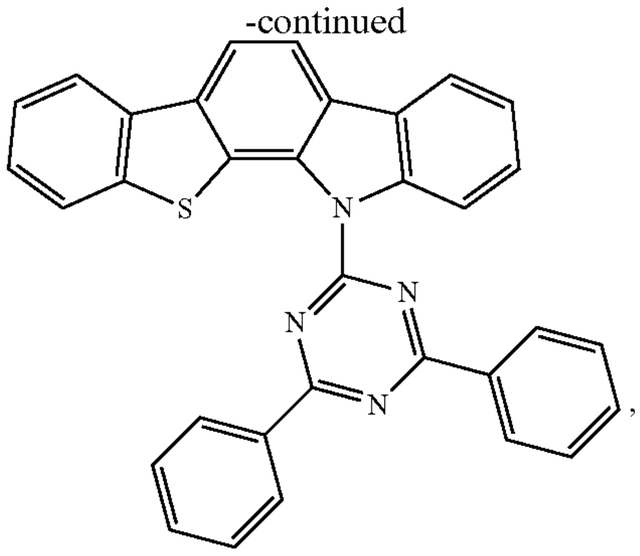
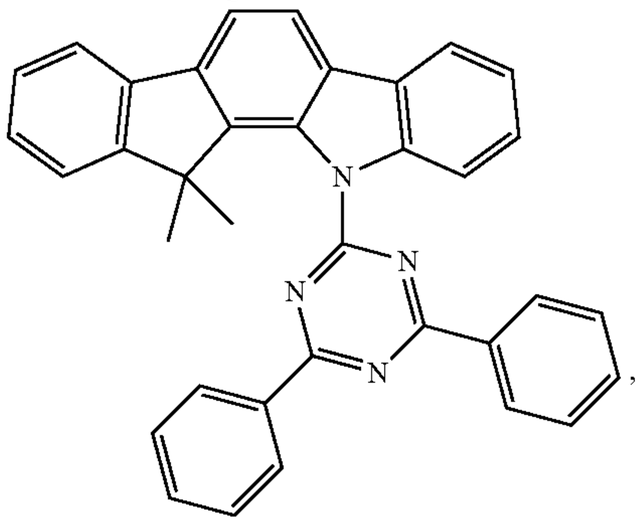
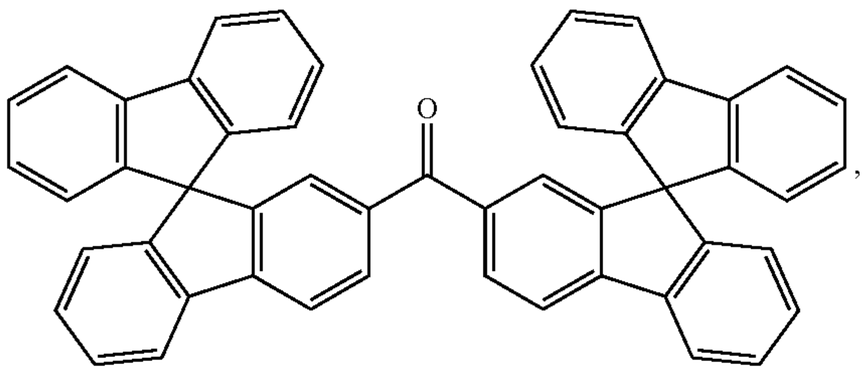
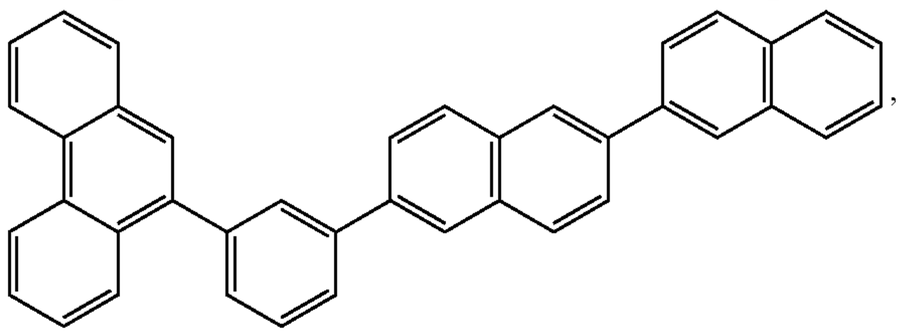
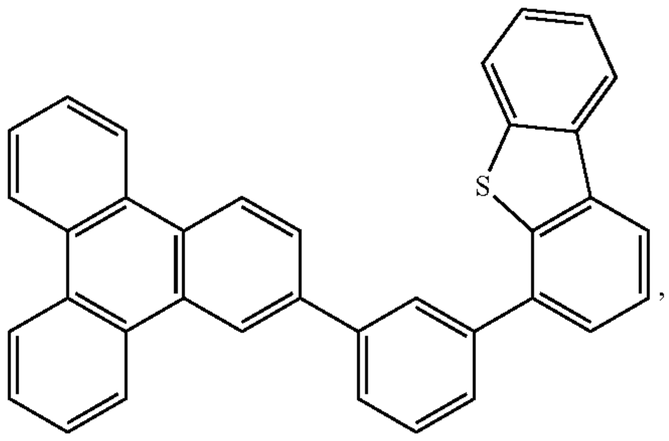
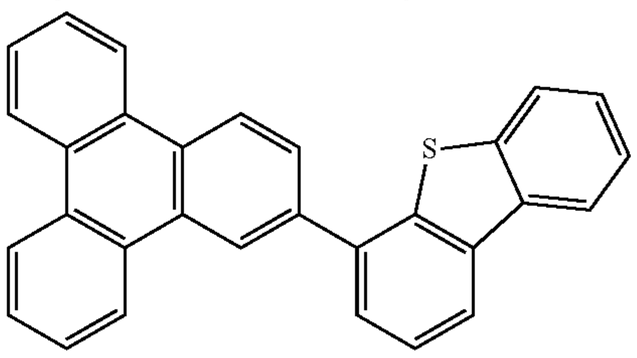












and combinations thereof.

In yet another aspect of the present disclosure, a formulation that includes a compound including L_1 coordinated to a metal M as described herein is described. In some embodiments, the formulation can include a compound of Formula II as described herein, and variations thereof. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, an electron transport layer material (see below).

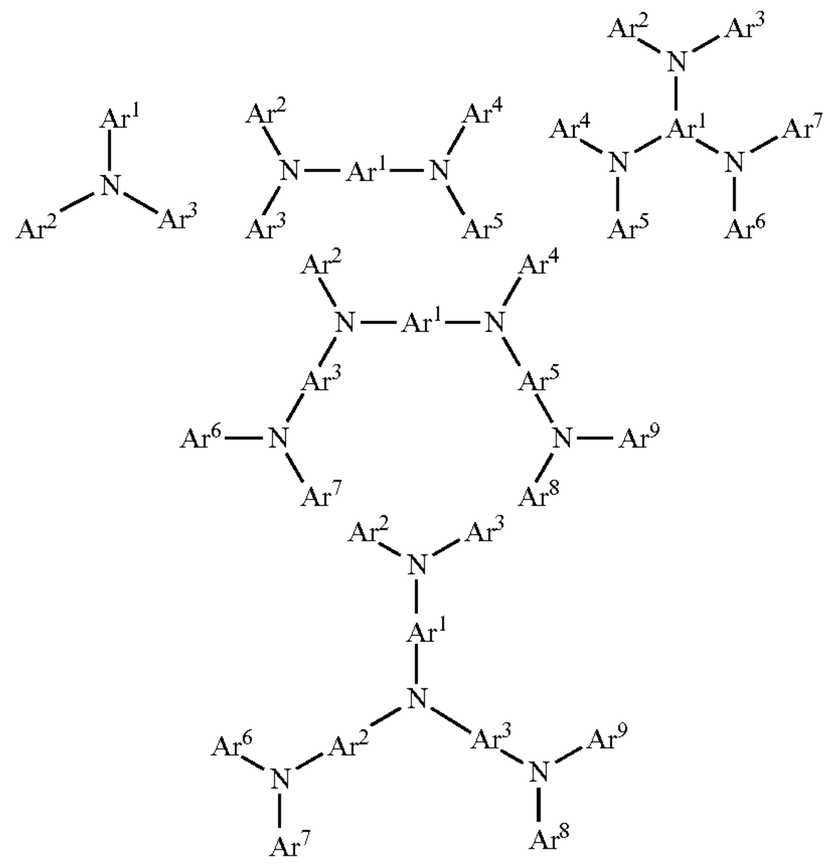
Combination with Other Materials

The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

HIL/HTL:

A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphryin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and sliane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

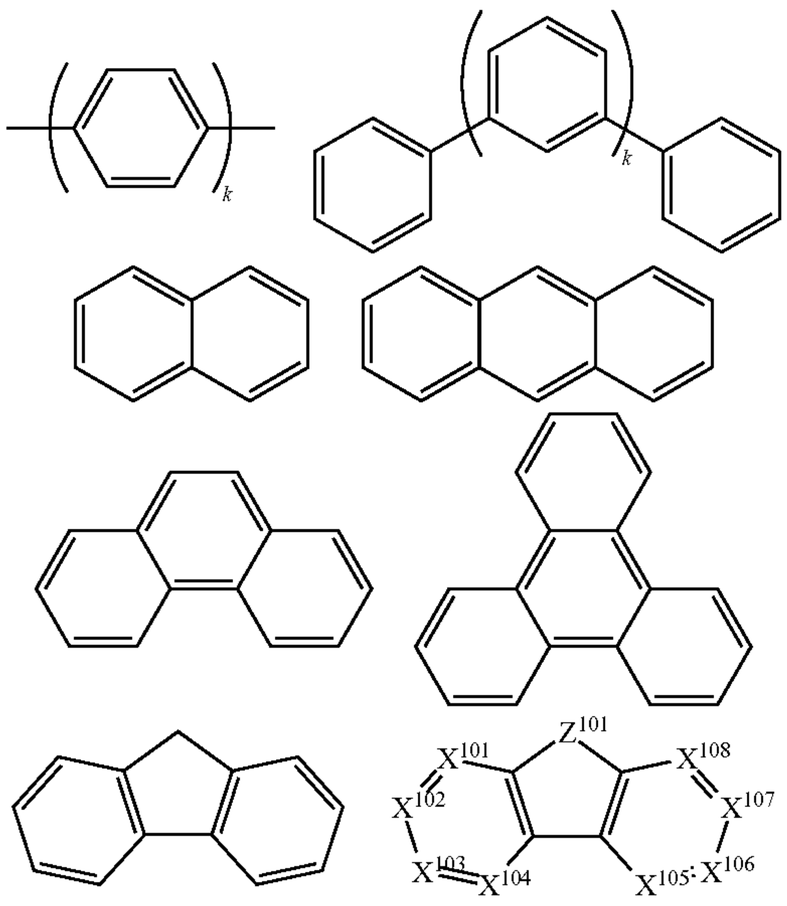
Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:



Each of Ar^1 to Ar^9 is selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, diben-

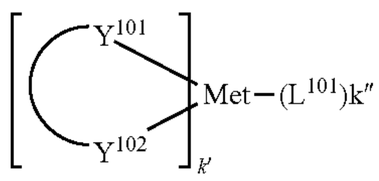
zoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

In one aspect, Ar^1 to Ar^9 is independently selected from the group consisting of:



k is an integer from 1 to 20; X^{101} to X^{108} is C (including CH) or N; Z^{101} is NAr^1, O, or S; Ar^1 has the same group defined above.

Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:



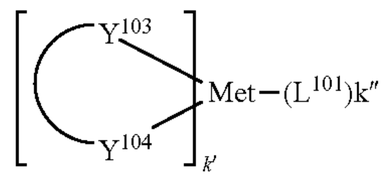
Met is a metal, which can have an atomic weight greater than 40; $(Y^{101}\text{-}Y^{102})$ is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L_{101} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

In one aspect, $(Y^{101}\text{-}Y^{102})$ is a 2-phenylpyridine derivative. In another aspect, $(Y^{101}\text{-}Y^{102})$ is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc^+/Fc couple less than about 0.6 V.

Host:

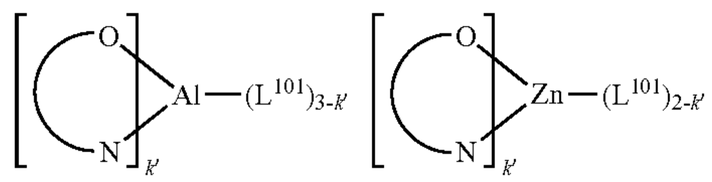
The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. While the Table below categorizes host materials as preferred for devices that emit various colors, any host material may be used with any dopant so long as the triplet criteria is satisfied.

Examples of metal complexes used as host are preferred to have the following general formula:



Met is a metal; $(Y^{103}\text{-}Y^{104})$ is a bidentate ligand, Y^{103} and Y^{104} are independently selected from C, N, O, P, and S; L^{101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

In one aspect, the metal complexes are:



(O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

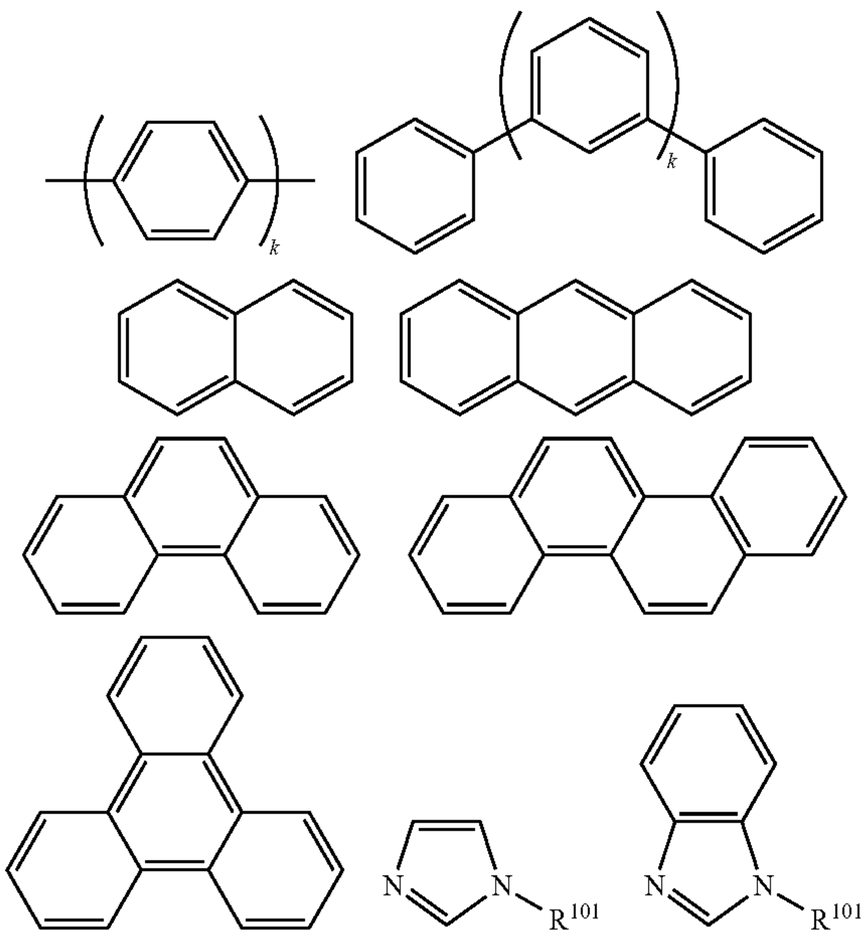
In another aspect, Met is selected from Ir and Pt.

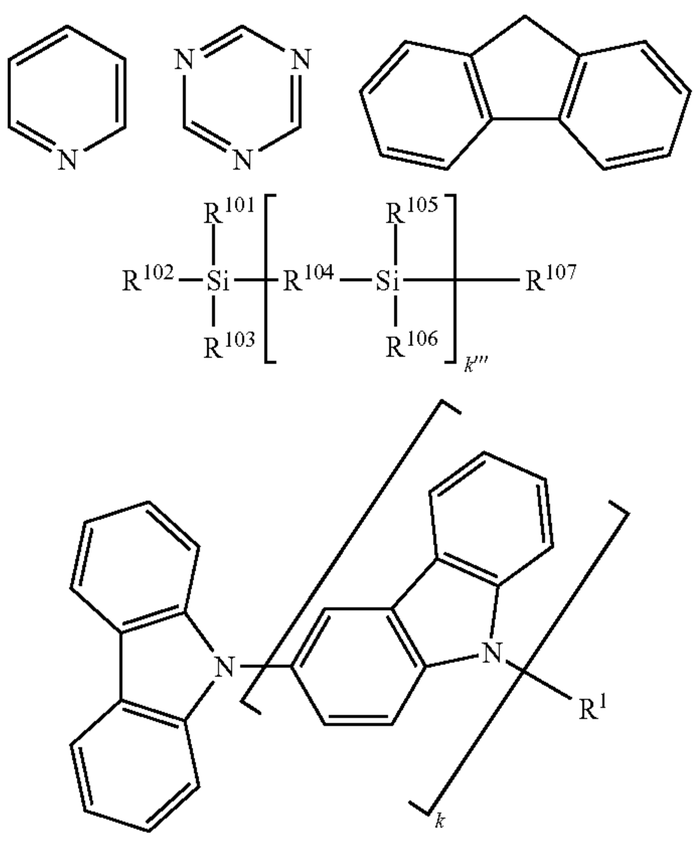
In a further aspect, $(Y^{103}\text{-}Y^{104})$ is a carbene ligand.

Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quino-

line, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

In one aspect, host compound contains at least one of the following groups in the molecule:





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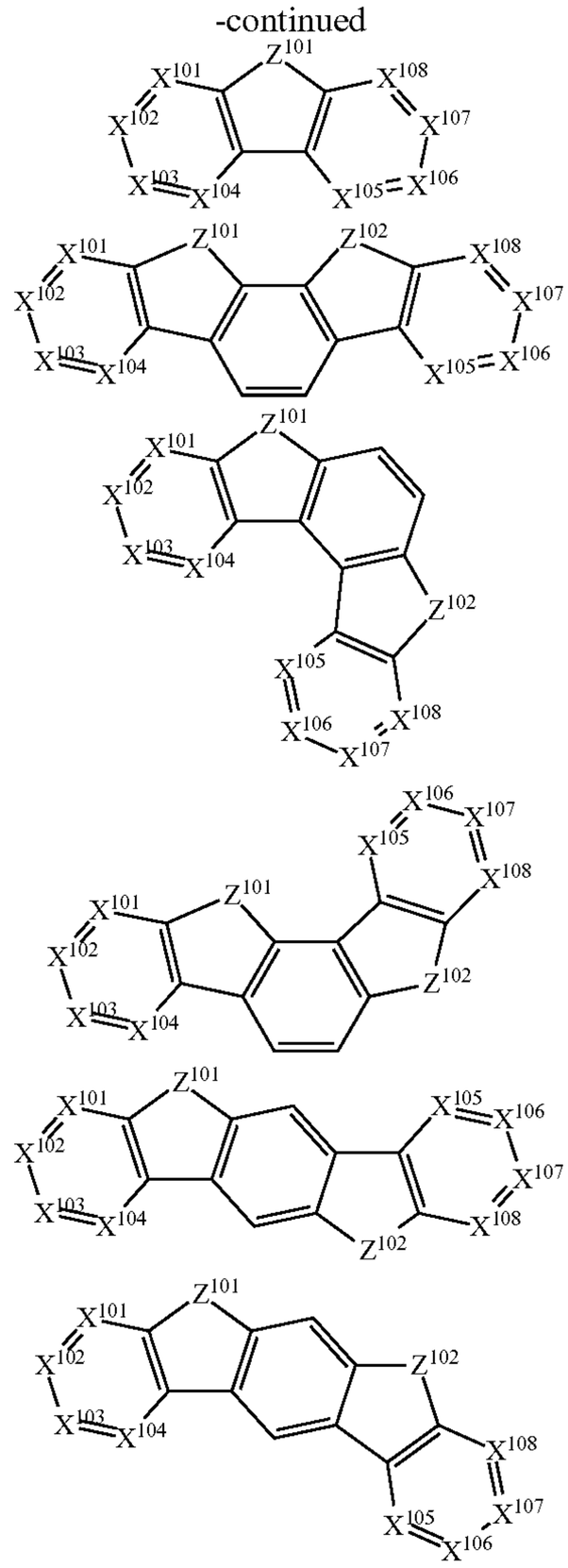


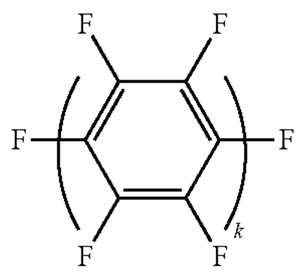
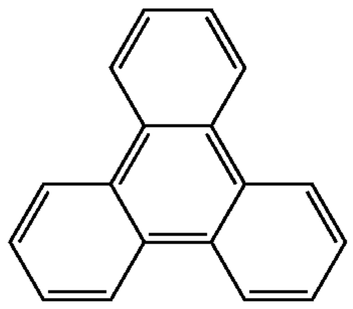
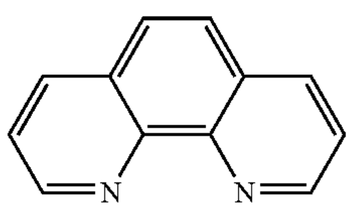
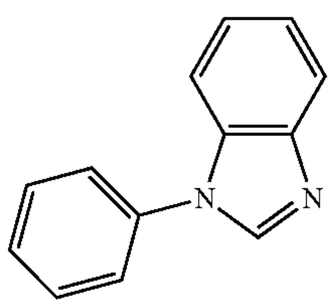
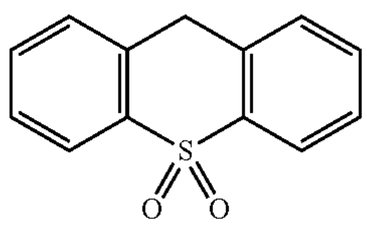
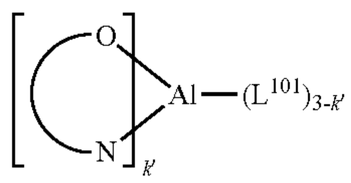
R^{101} to R^{107} is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

k is an integer from 0 to 20 or 1 to 20; k''' is an integer from 0 to 20. X^{101} to X^{108} is selected from C (including CH) or N. Z^{101} and Z^{102} is selected from NR^{101}, O, or S.

HBL:

A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above. In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

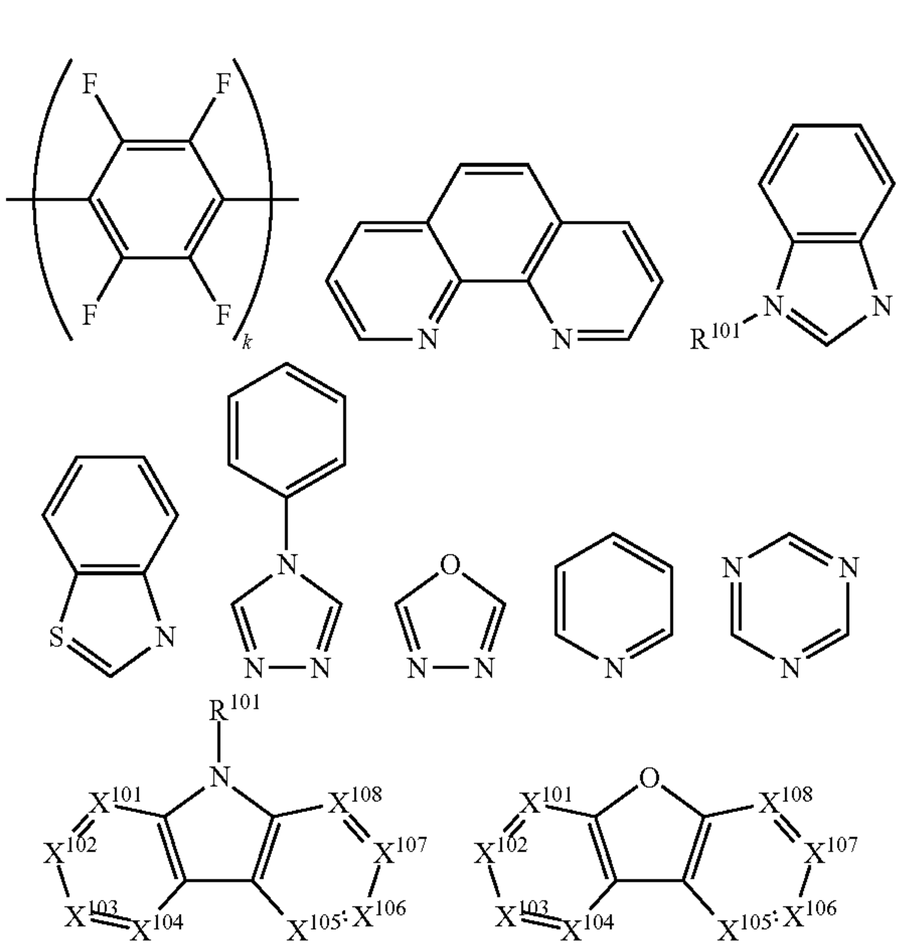







k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

In one aspect, compound used in ETL contains at least one of the following groups in the molecule:



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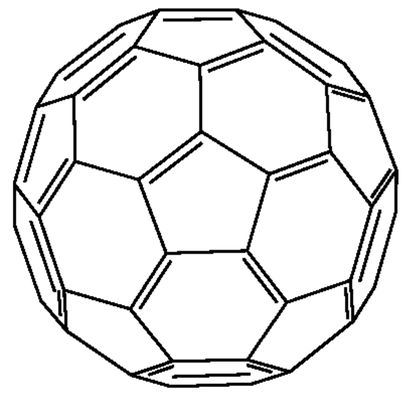
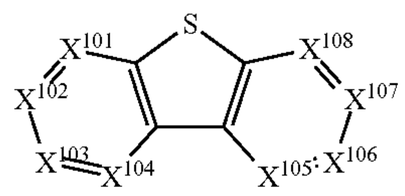
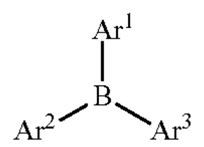
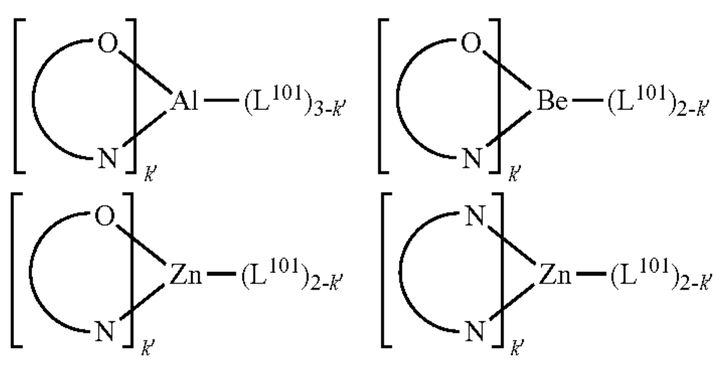




R^{101} is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above.

Ar^1 to Ar^1 has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X^{101} to X^{108} is selected from C (including CH) or N.

In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:



(O—N) or (N—N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{101} is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. encompasses undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also encompass undeuterated, partially deuterated, and fully deuterated versions thereof.

In addition to and/or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 1 below. Table 1 lists non-limiting classes of materials, non-limiting examples of compounds for each-class, and references that disclose the materials.

TABLE 1

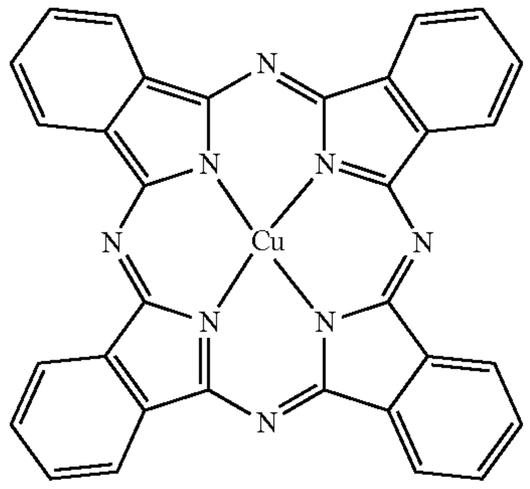
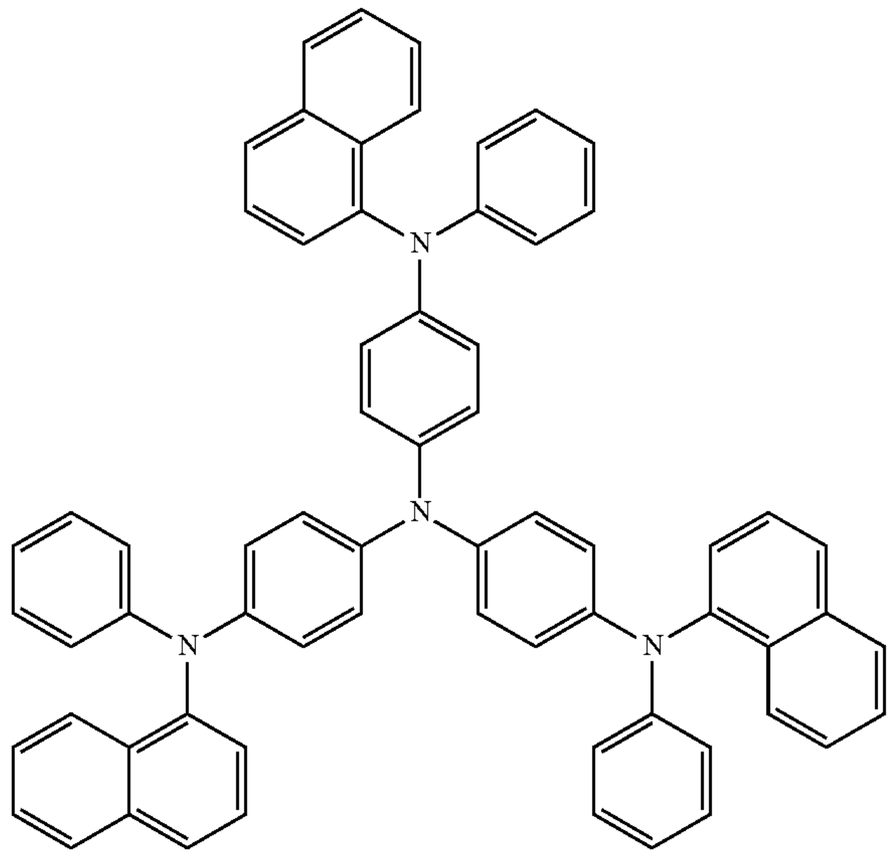
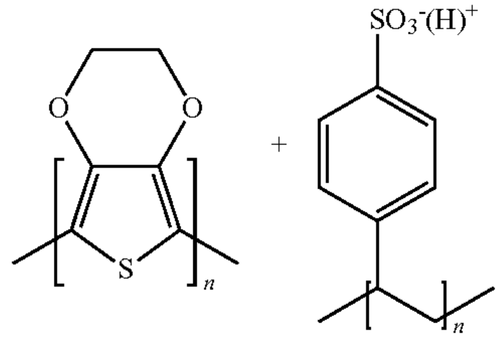
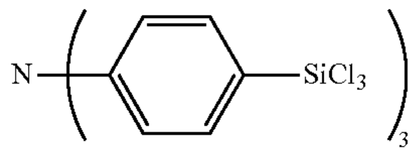
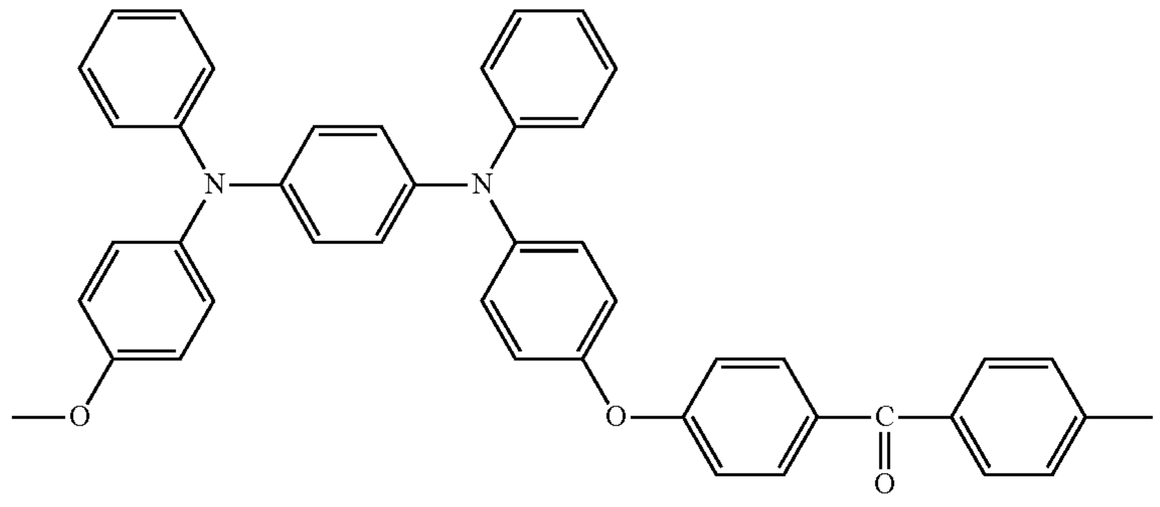
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Hole injection materials	
Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)
Starburst tri-arylamines		J. Lumin. 72-74, 985 (1997)
CF_x Fluorohydro-carbon polymer	$-[CH_xF_y]_n-$	Appl. Phys. Lett. 78, 673 (2001)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)		Synth. Met. 87, 171 (1997) WO2007002683
Phosphonic acid and sliane SAMs		US20030162053
Triarylamine or polythiophene polymers with conductivity dopants		EP1725079A1

and

TABLE 1-continued

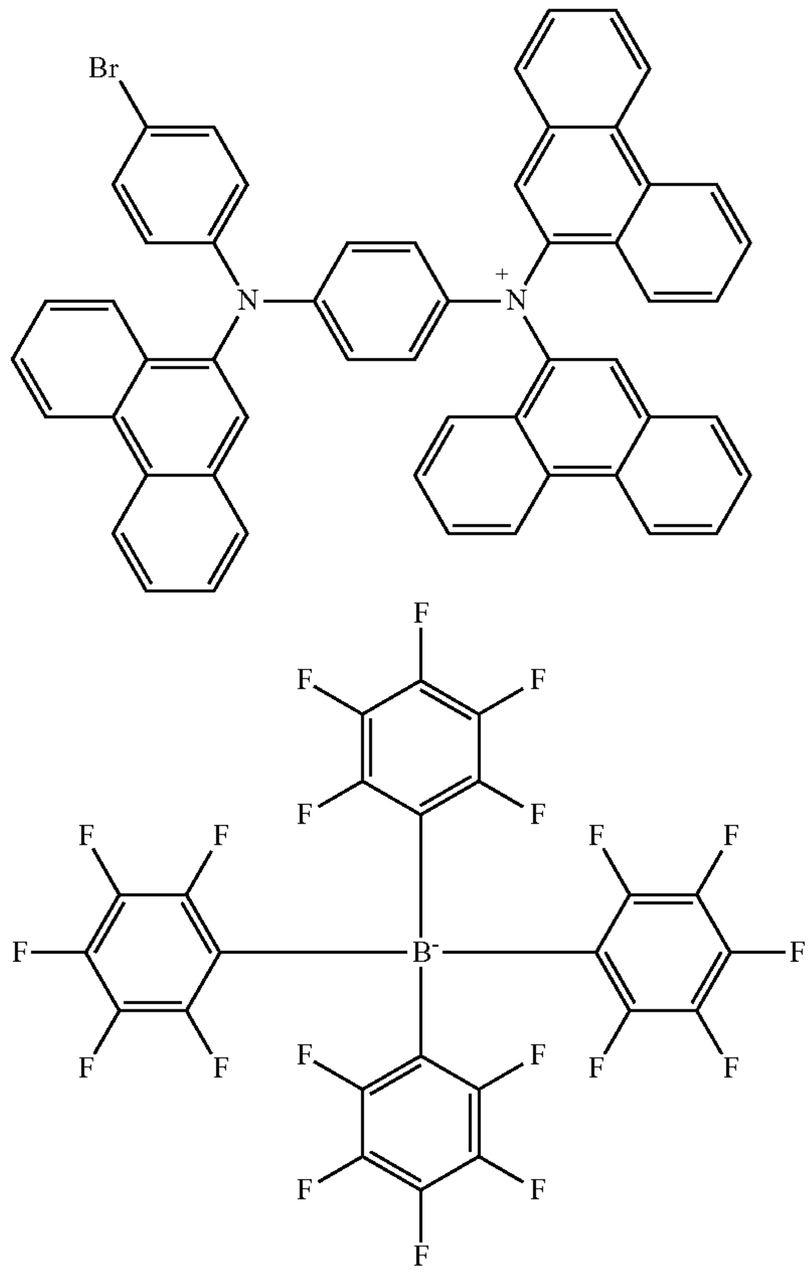
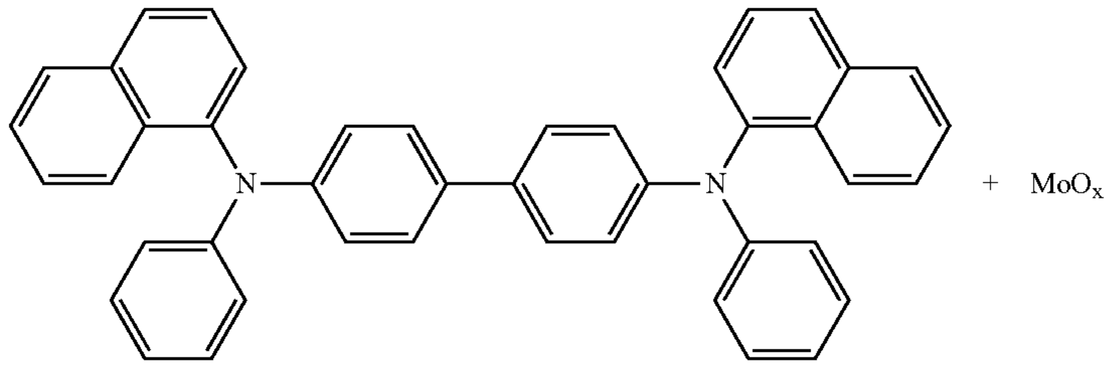
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		
Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides		US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009

TABLE 1-continued

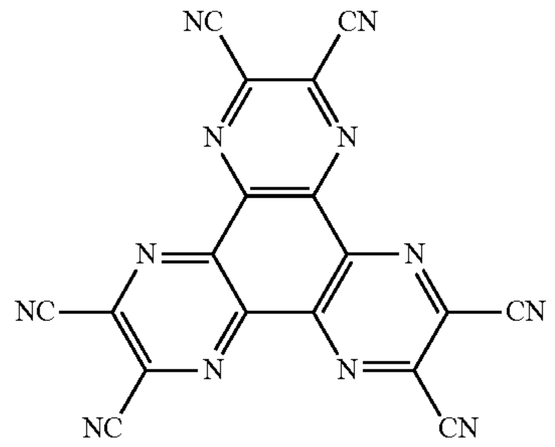
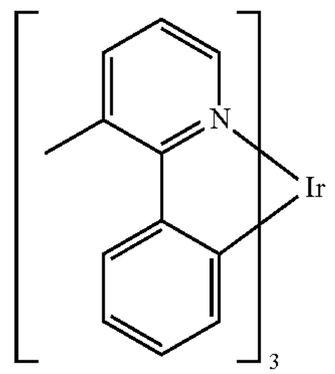
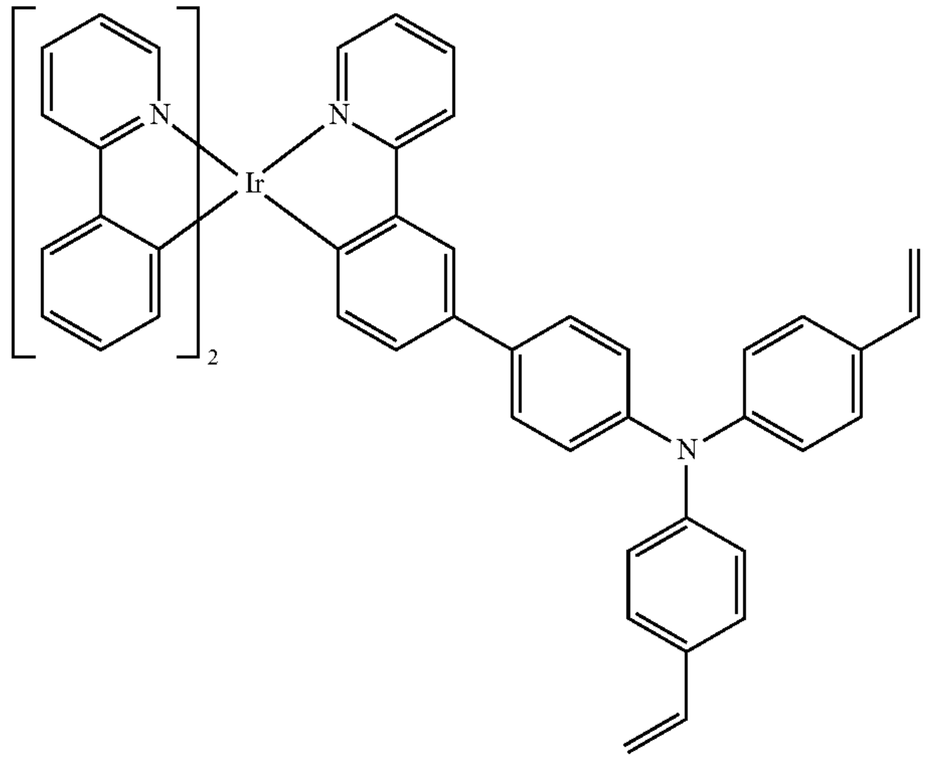
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
n-type semi-conducting organic complexes		US20020158242
Metal organo-metallic complexes		US20060240279
Cross-linkable compounds		US20080220265

TABLE 1-continued

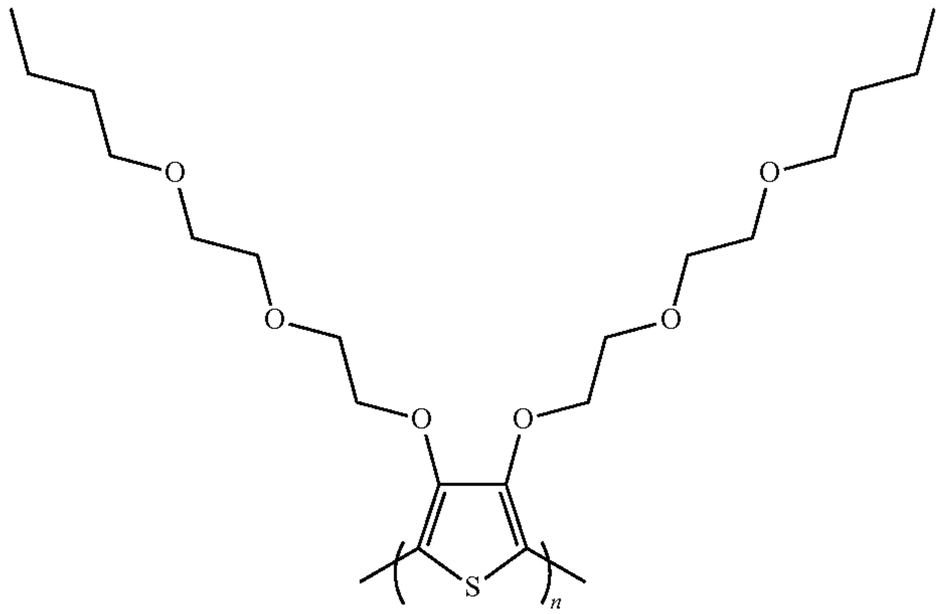
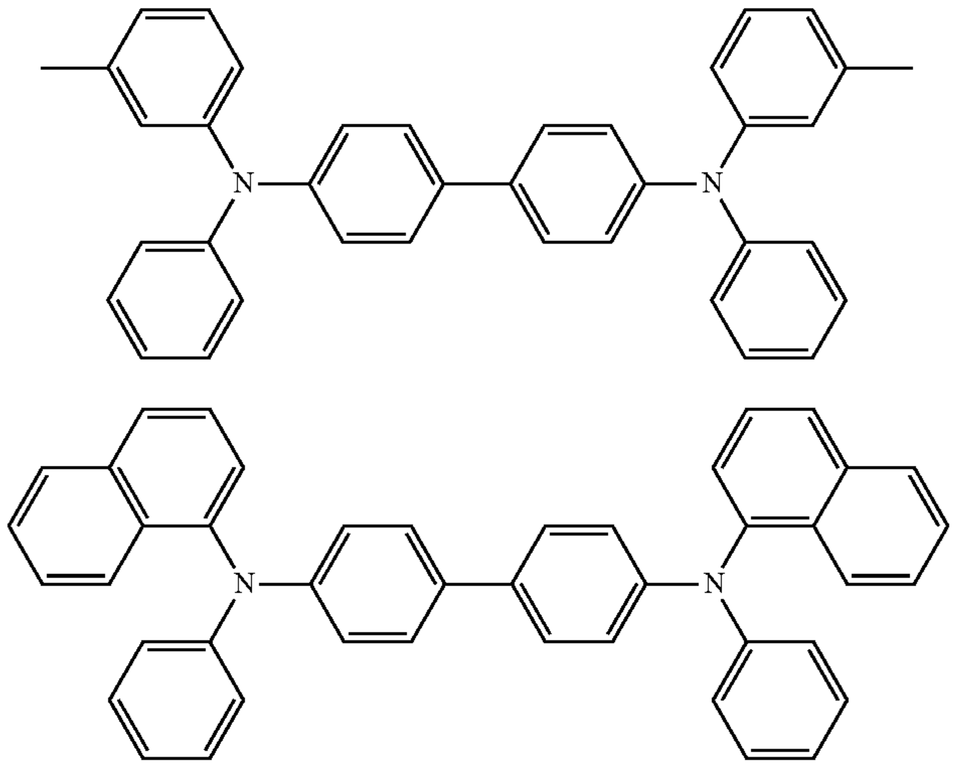
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Polythiophene based polymers and copolymers		WO 201105644 EP2350216
Hole transporting materials		
Triarylamines (e.g., TPD, α-NPD)		Appl. Phys. Lett. 51, 913 (1987) US5061569

TABLE 1-continued

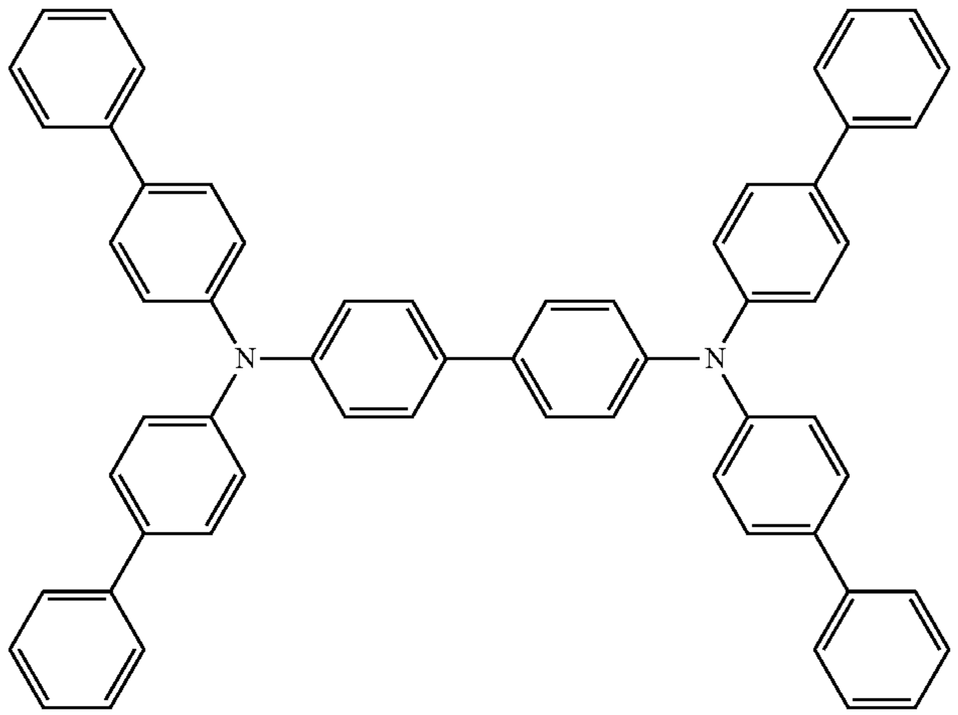
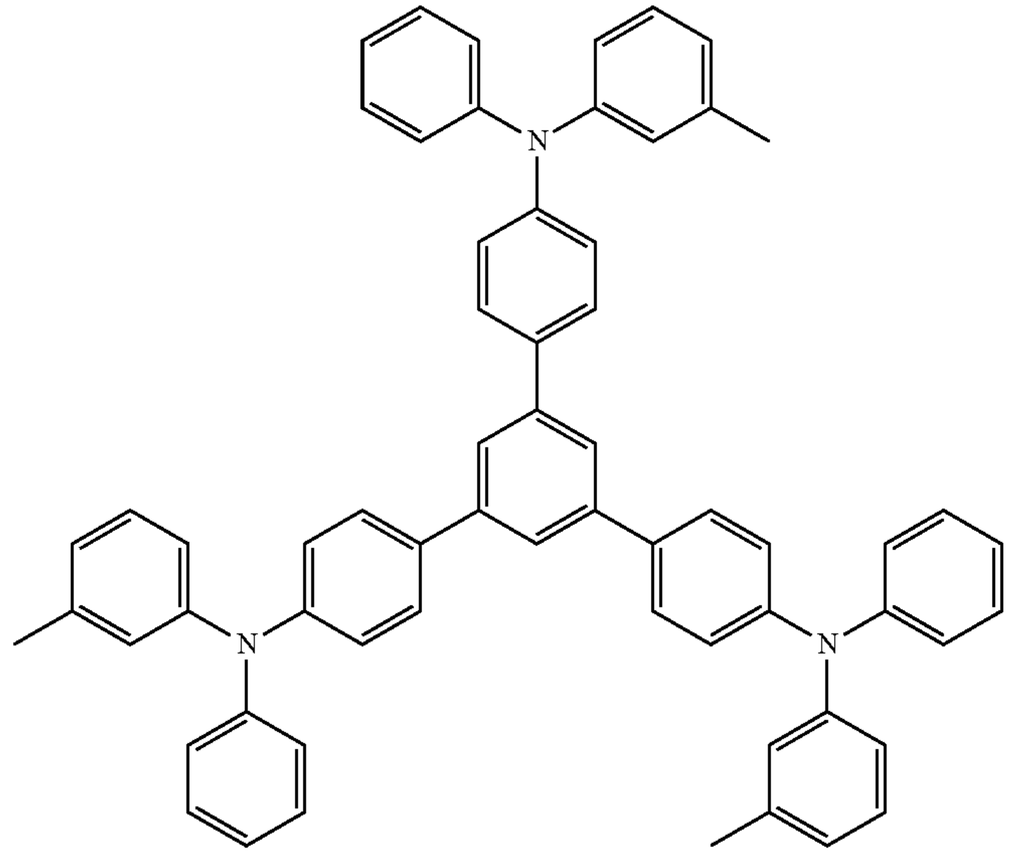
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		EP650955
		J. Mater. Chem. 3, 319 (1993)

TABLE 1-continued

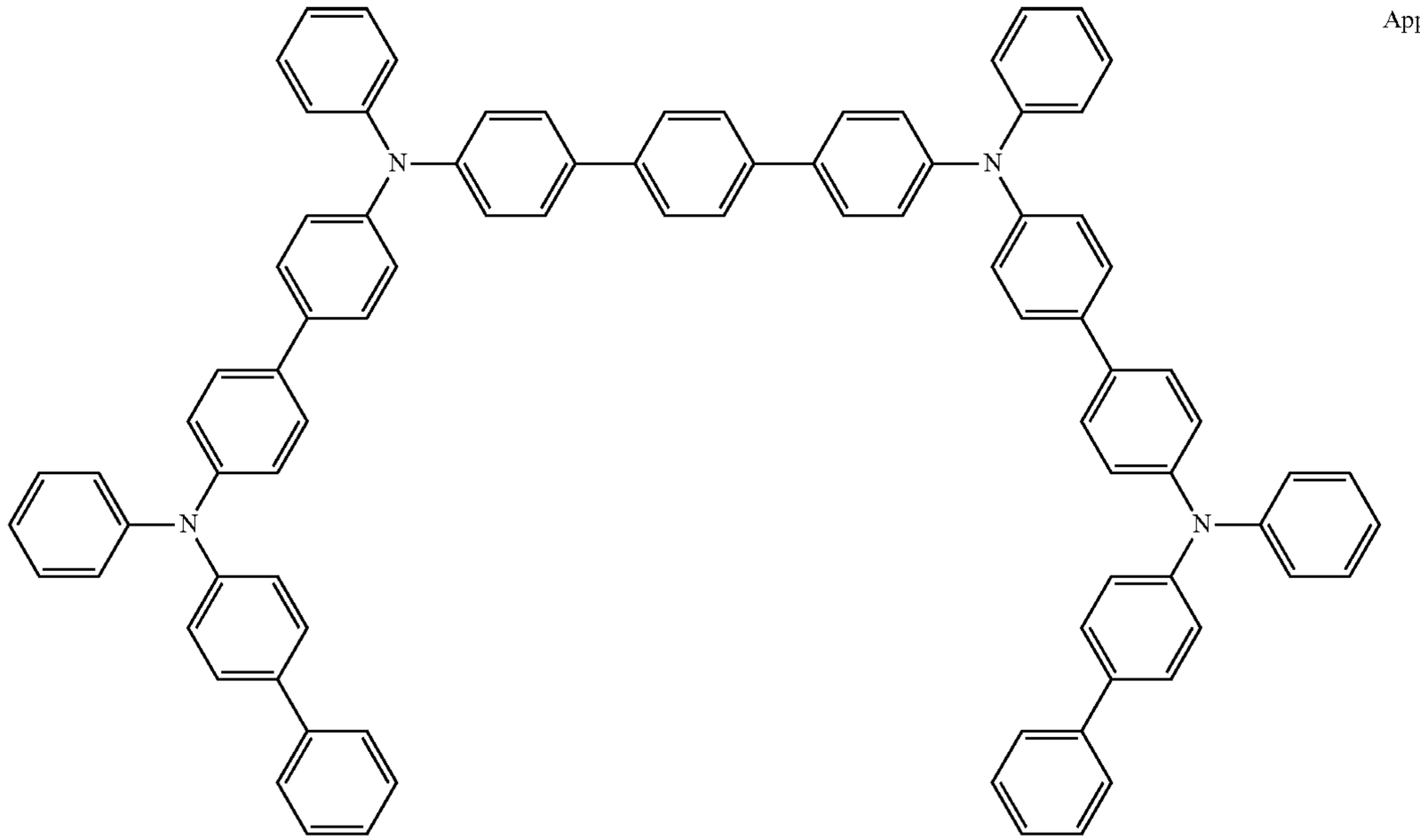
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)

TABLE 1-continued

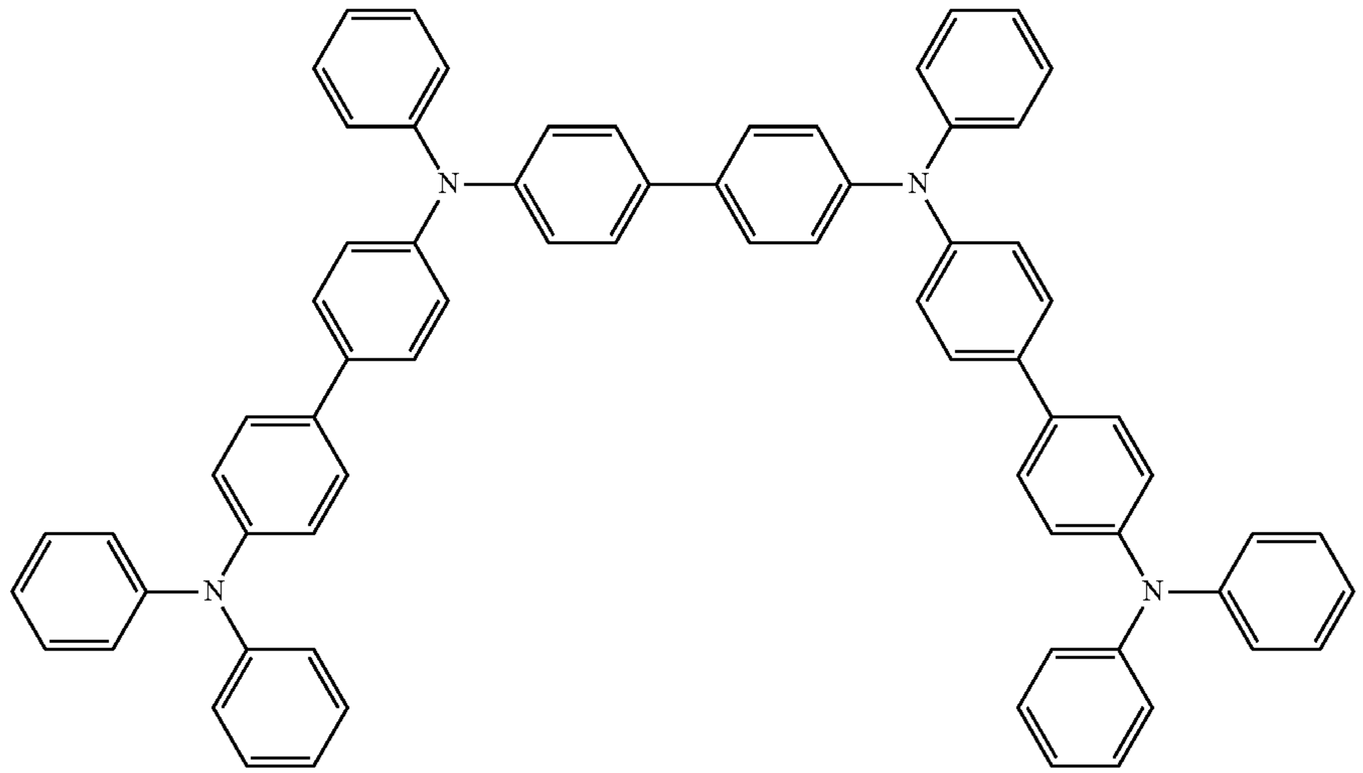
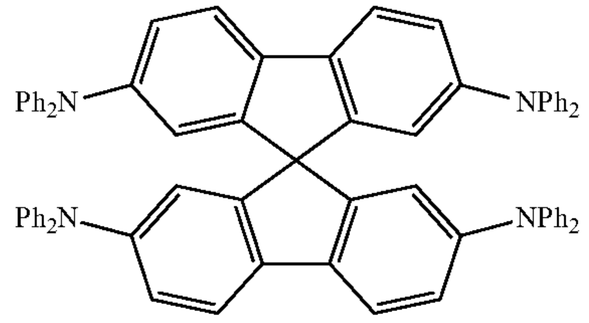
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 90, 183503 (2007)
Triaylamine on spirofluorene core		Synth. Met. 91, 209 (1997)

TABLE 1-continued

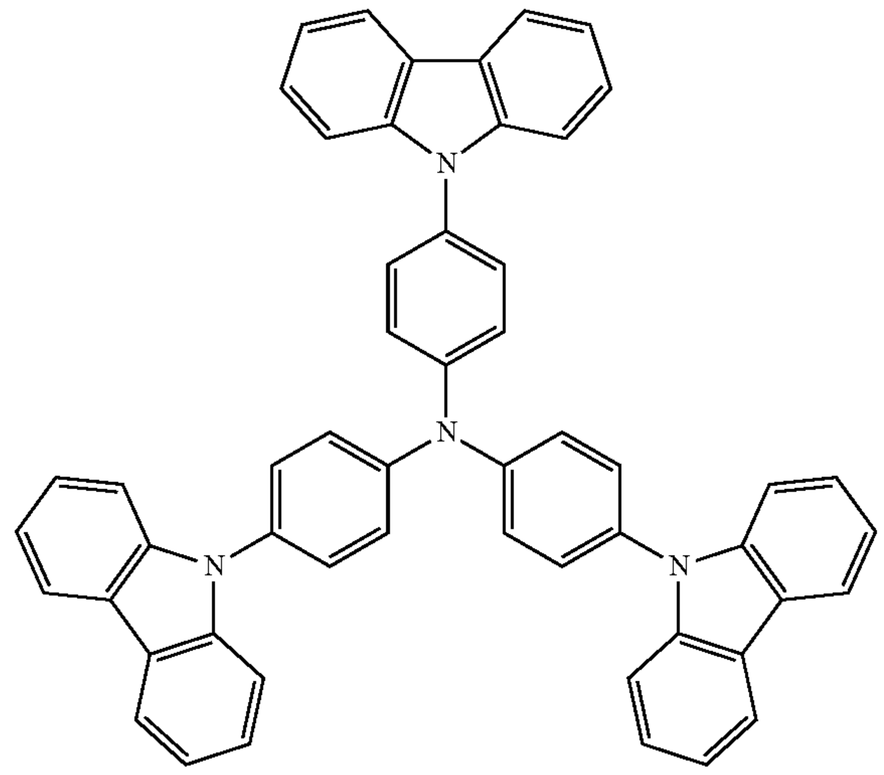
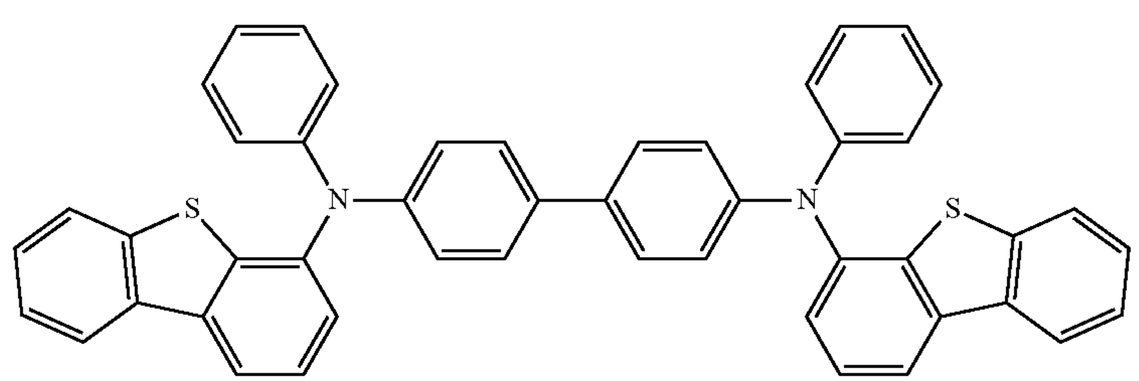
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
Triarylamine with (di)benzo-thiophene/ (di)benzofuran		US20070278938, US20080106190 US20110163302

TABLE 1-continued

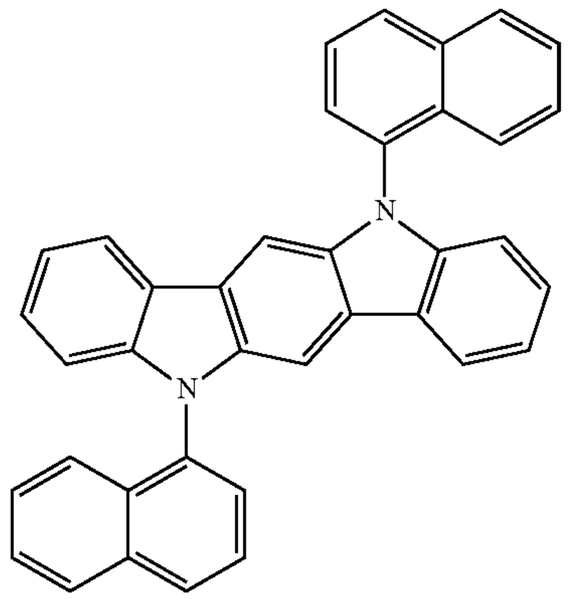
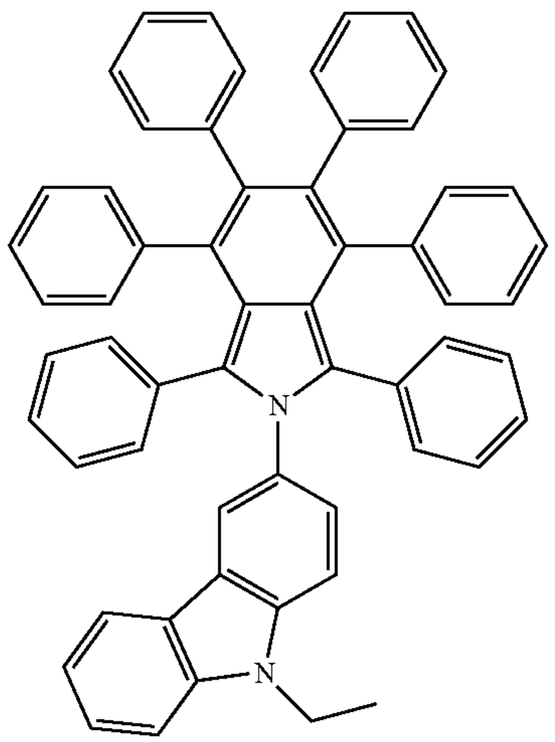
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocarbazoles		Synth. Met. 111, 421 (2000)
Isoindole compounds		Chem. Mater. 15, 3148 (2003)

TABLE 1-continued

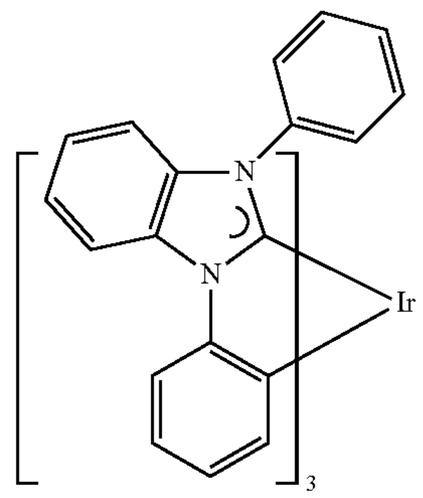
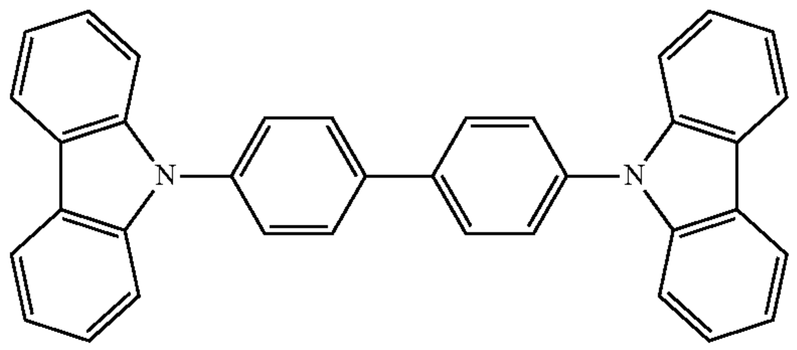
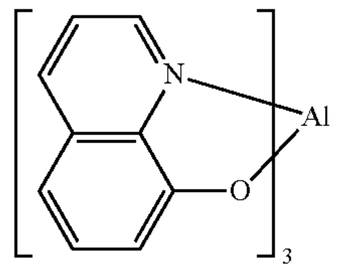
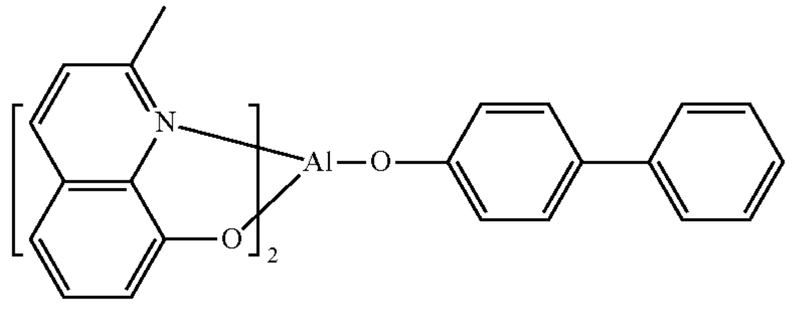
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal carbene complexes		US20080018221
	Phosphorescent OLED host materials Red hosts	
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
Metal 8-hydroxy-quinolates (e.g., Alq_3, BAlq)		Nature 395, 151 (1998)
		US20060202194

TABLE 1-continued

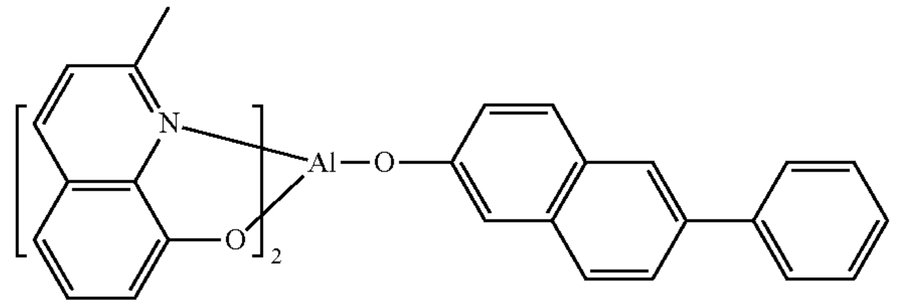
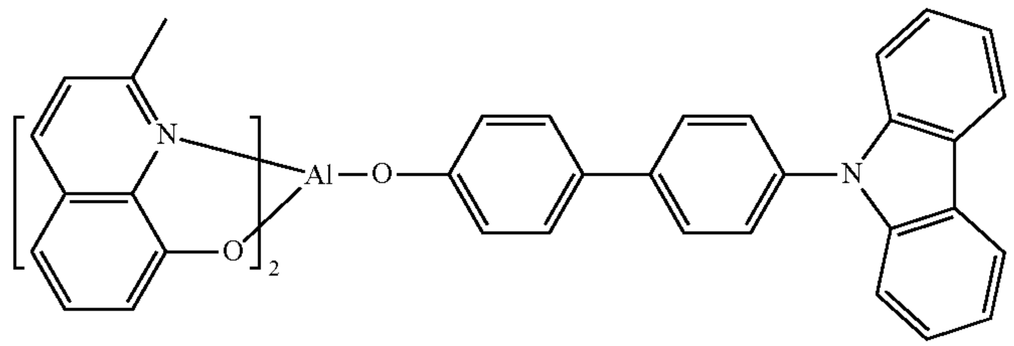
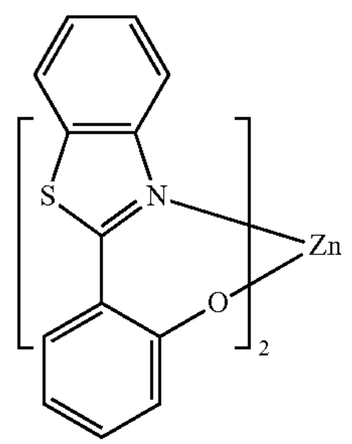
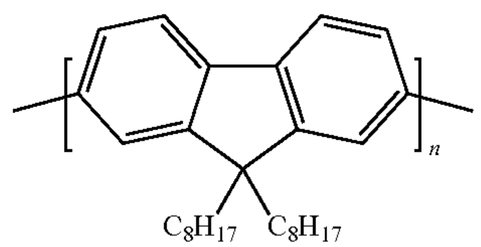
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005014551
		WO2006072002
Metal phenoxy-benzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)
Conjugated oligomers and polymers (e.g., polyfluorene)		Org. Electron. 1, 15 (2000)

TABLE 1-continued

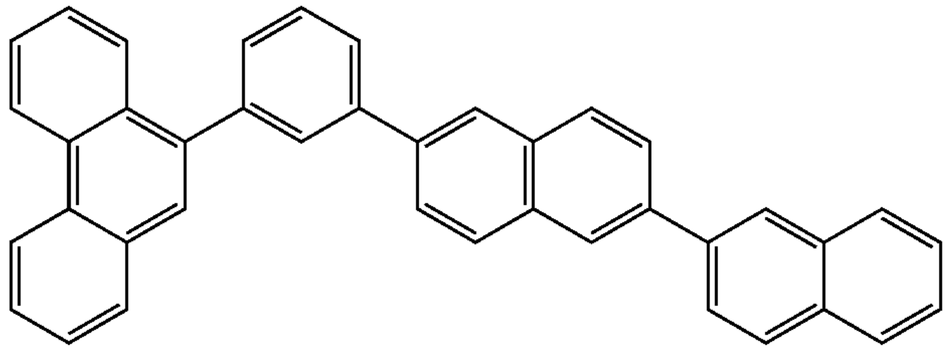
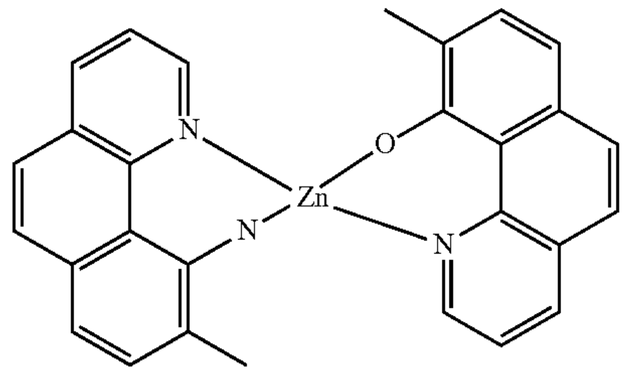
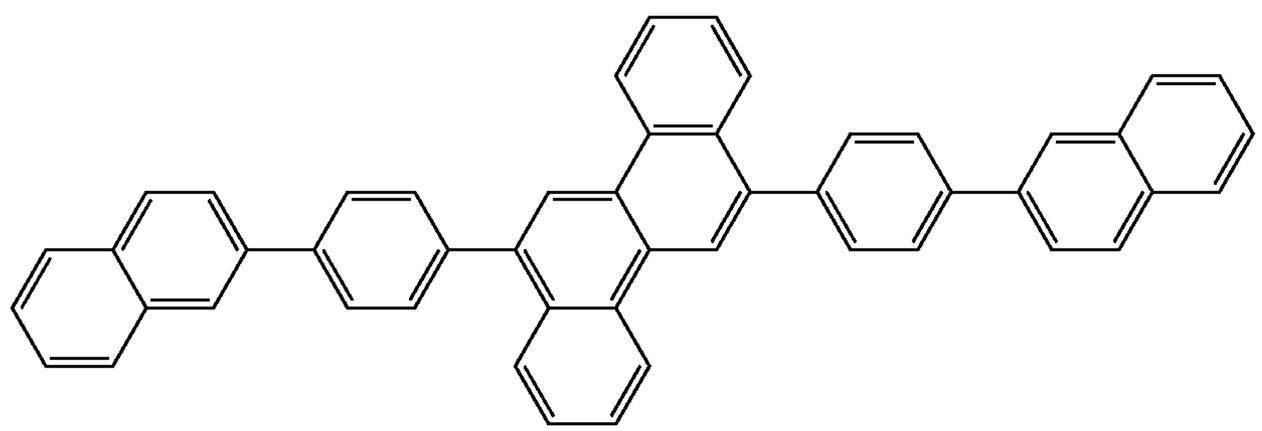
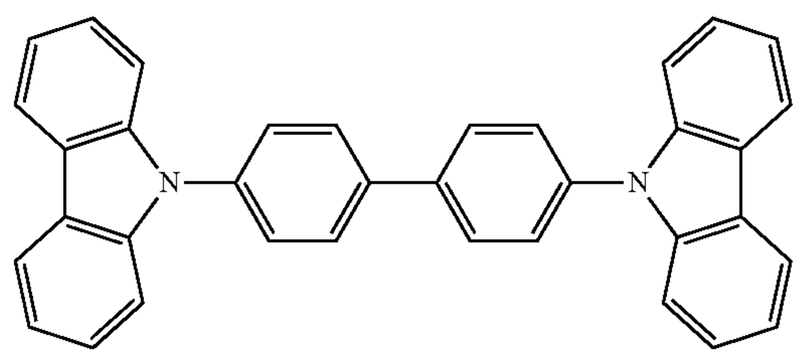
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
Zinc complexes		WO2010056066
Chrysene based compounds		WO2011086863
Green hosts		
Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

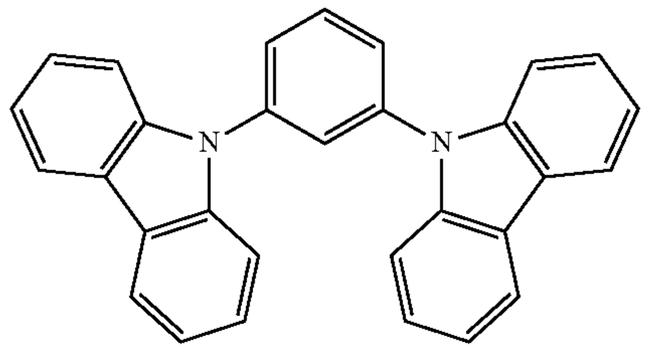
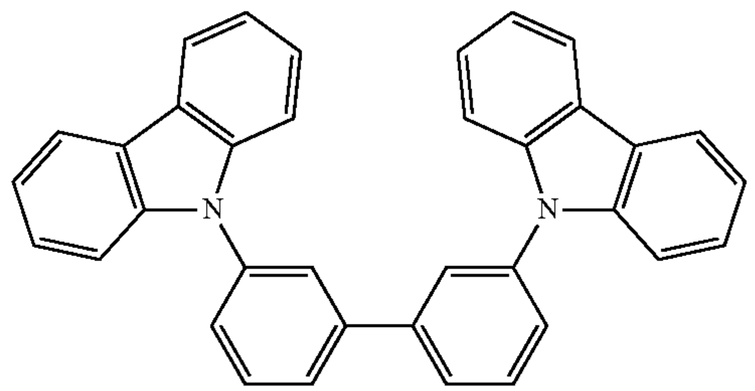
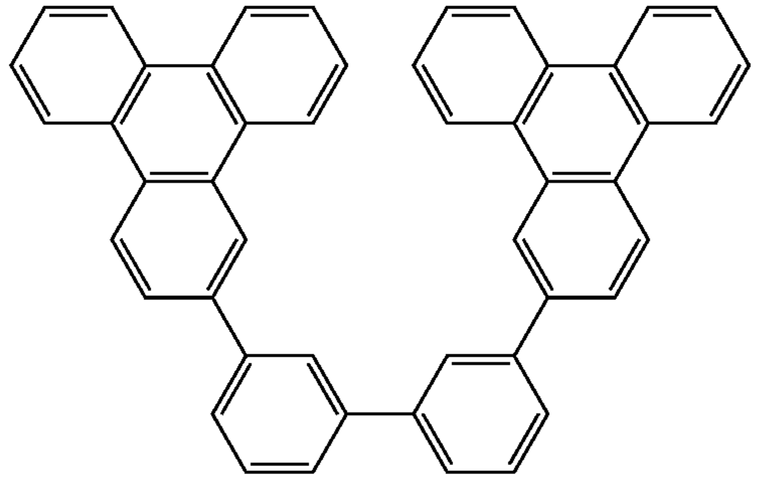
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20030175553
		WO2001039234
Aryltriphenylene compounds		US20060280965

TABLE 1-continued

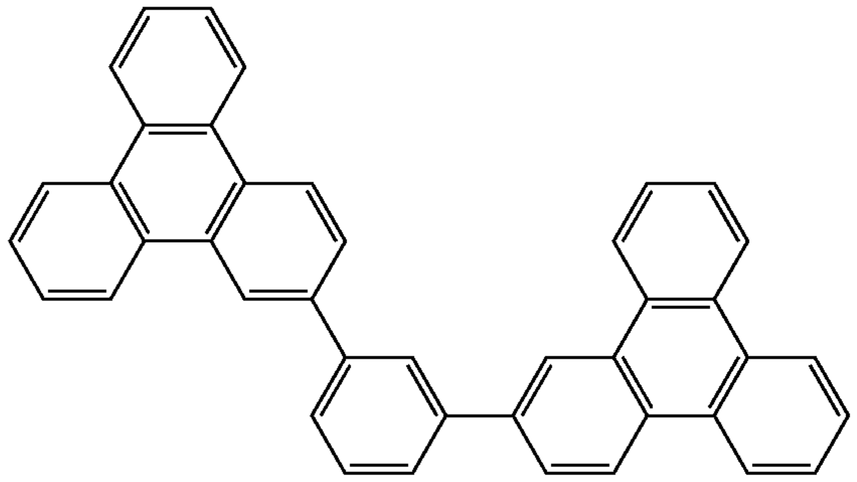
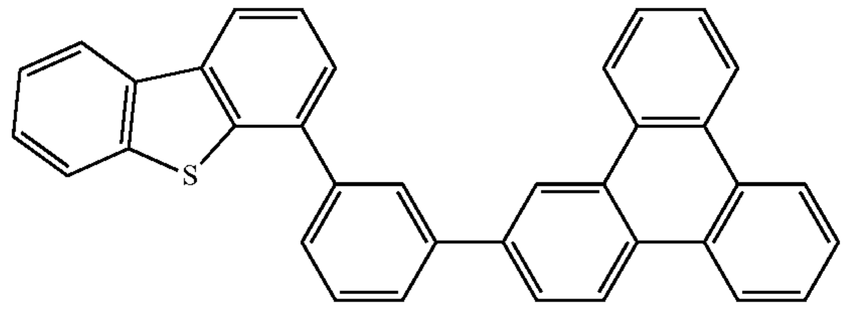
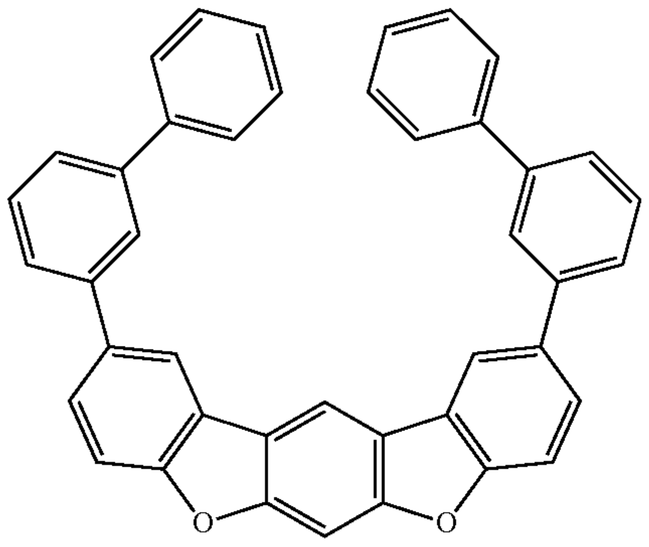
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060280965
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931

TABLE 1-continued

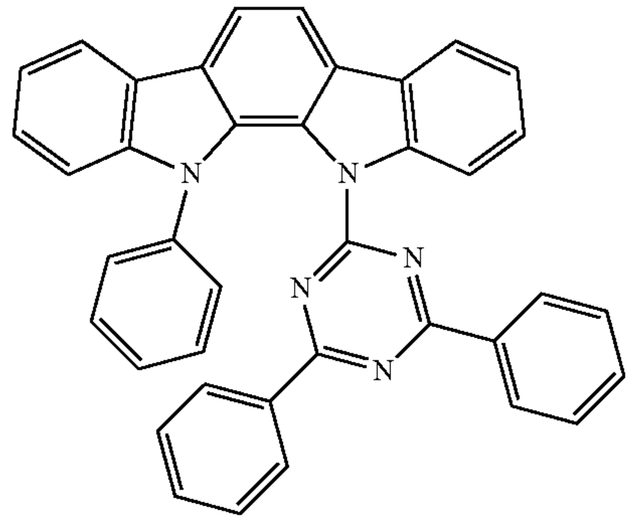
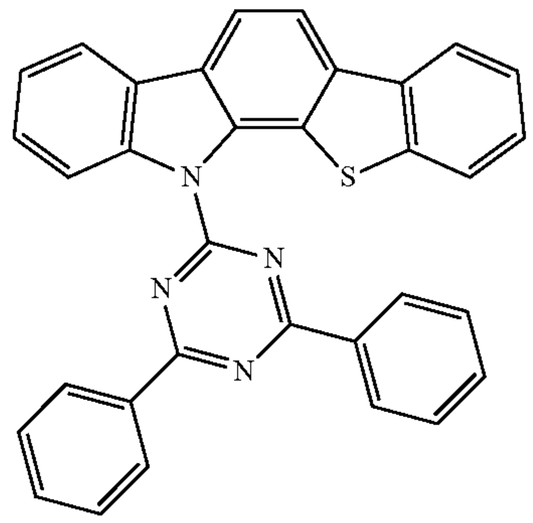
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Donor acceptor type molecules		WO2008056746
		WO2010107244

TABLE 1-continued

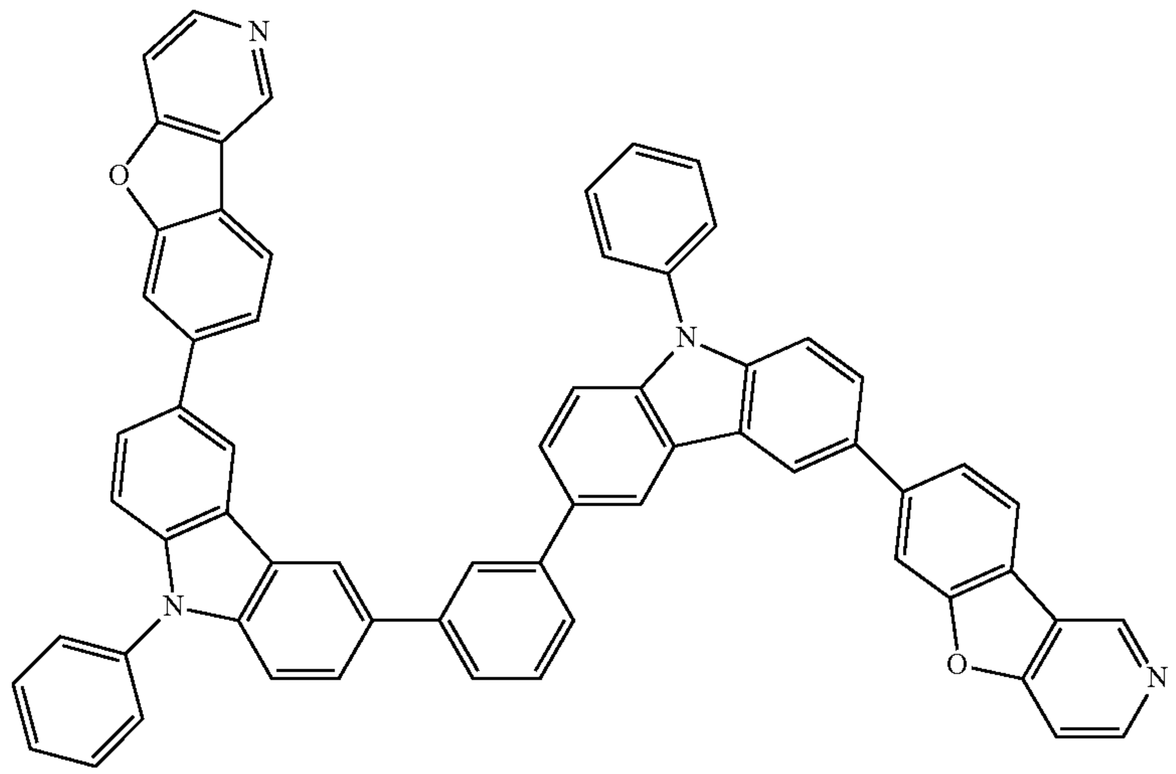
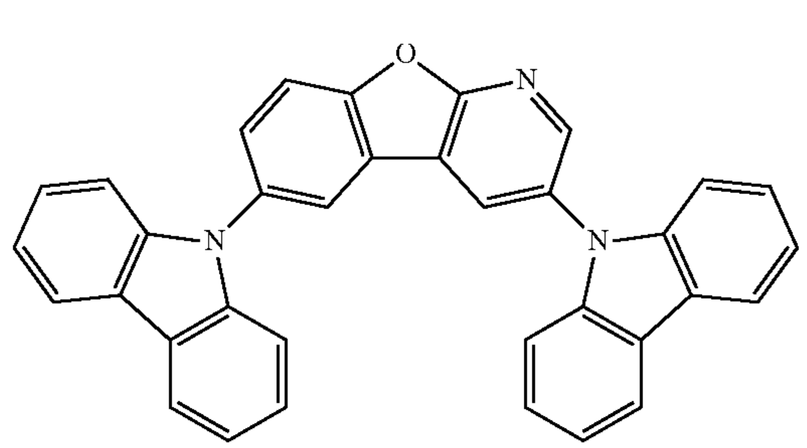
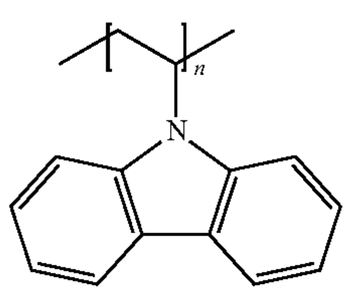
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Aza-carbazole/ DBT/DBF		JP2008074939
		US20100187984
Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)

TABLE 1-continued

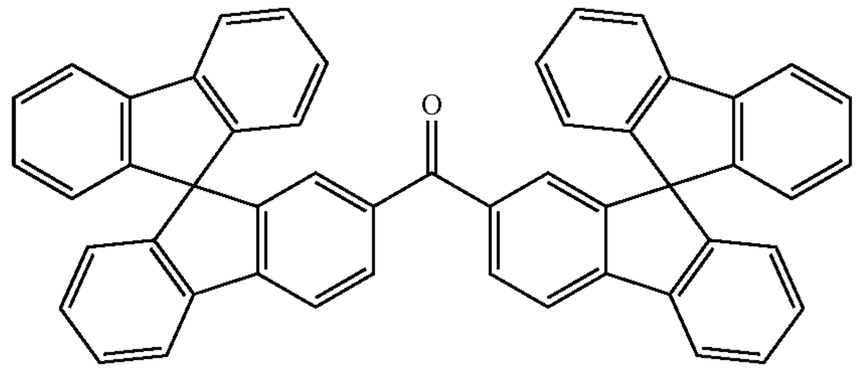
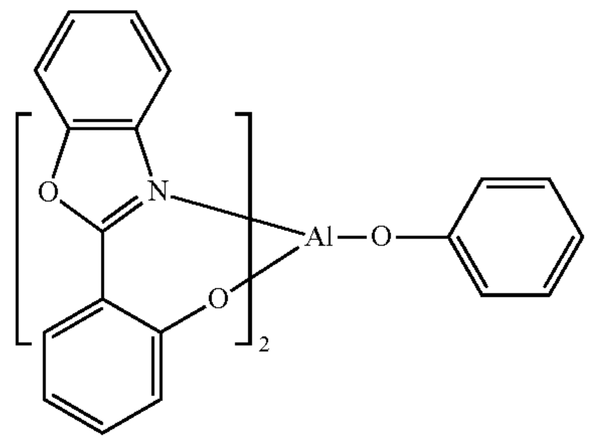
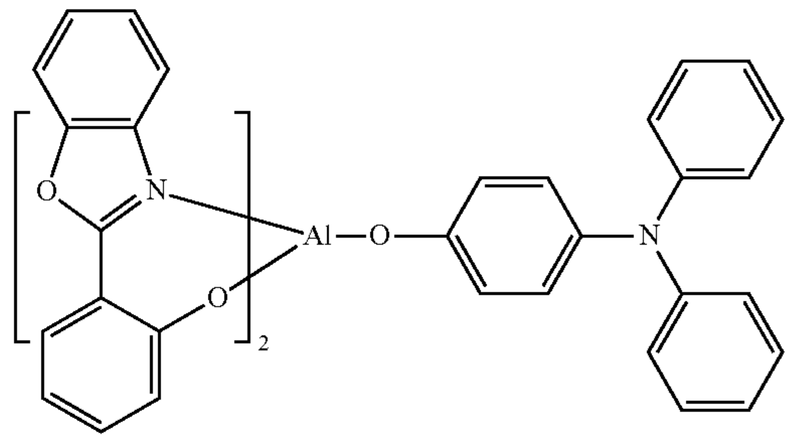
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Spirofluorene compounds		WO2004093207
Metal phenoxy-benzooxazole compounds		WO2005089025
		WO2006132173

TABLE 1-continued

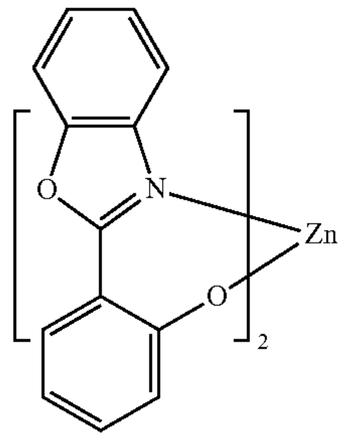
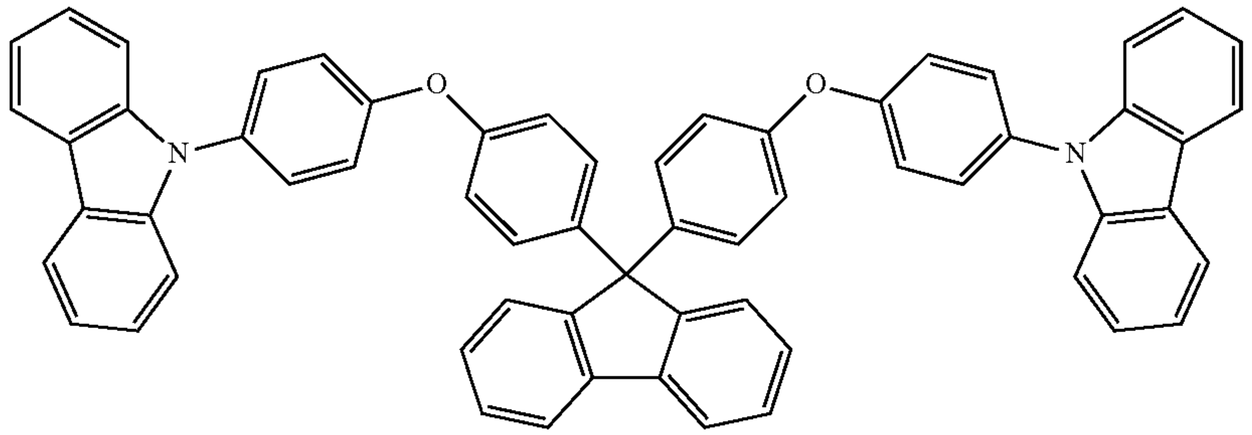
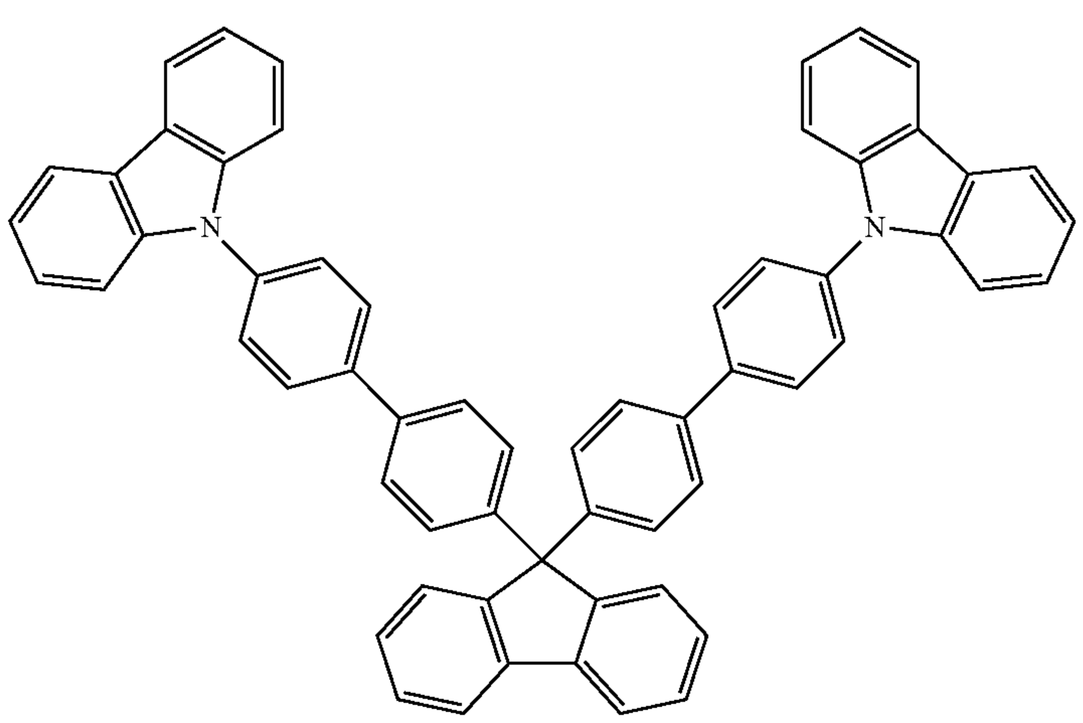
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		JP200511610
Spirofluorene-carbazole compounds		JP2007254297
		JP2007254297

TABLE 1-continued

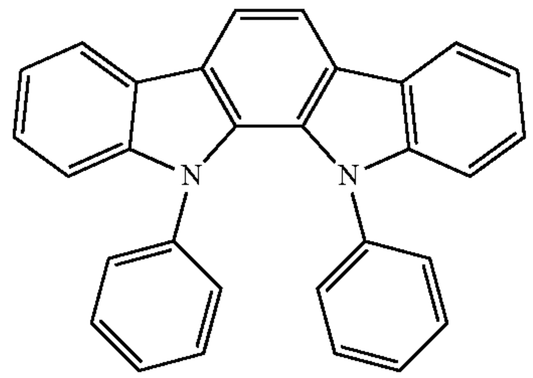
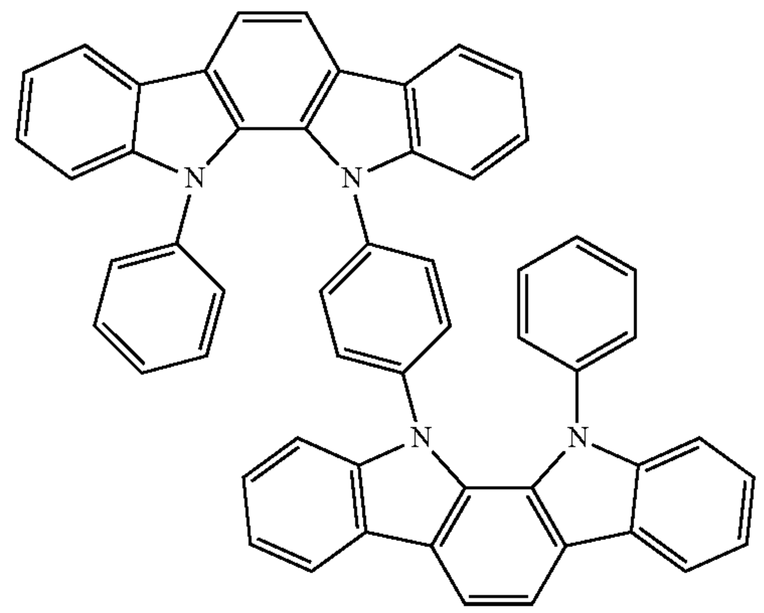
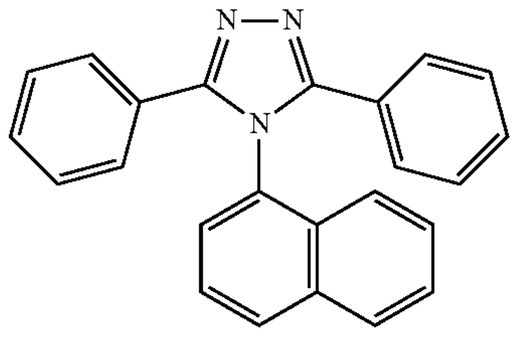
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Indolocabazoles		WO2007063796
		WO2007063754
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)

TABLE 1-continued

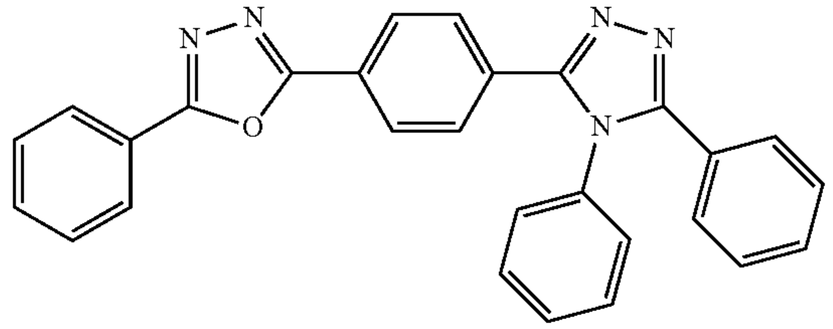
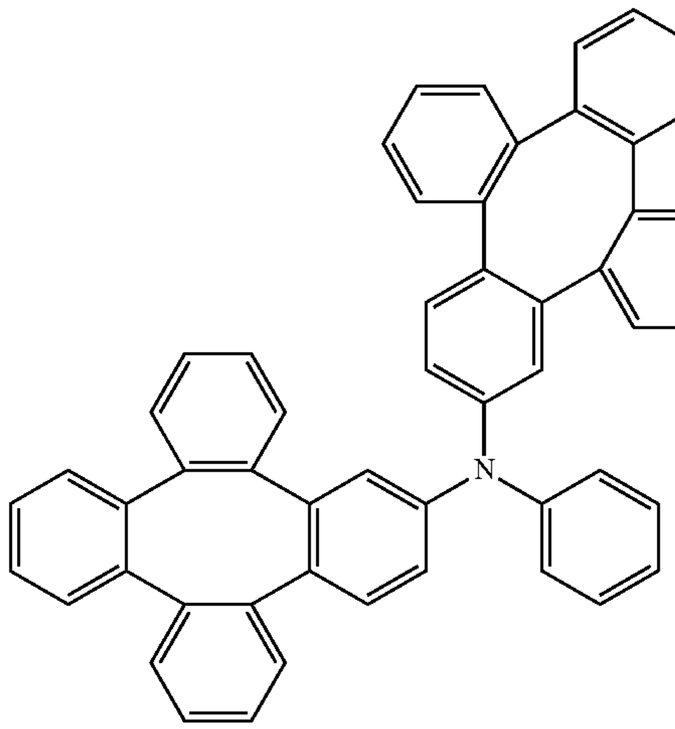
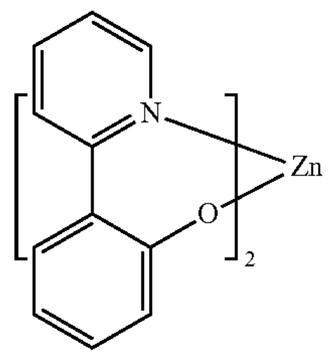
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2004107822
Tetraphenylene complexes		US20050112407
Metal phenoxy-pyridine compounds		WO2005030900

TABLE 1-continued

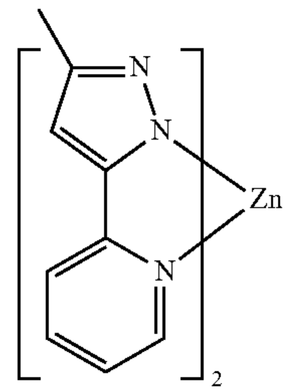
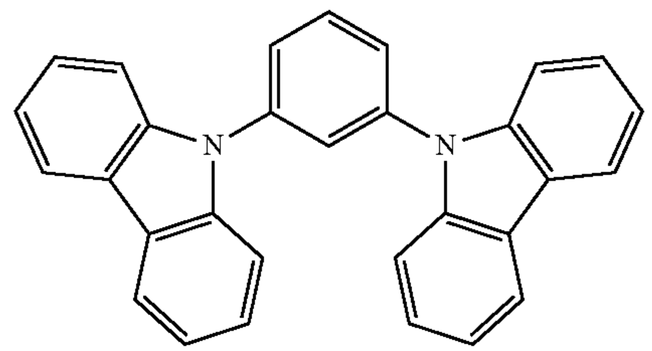
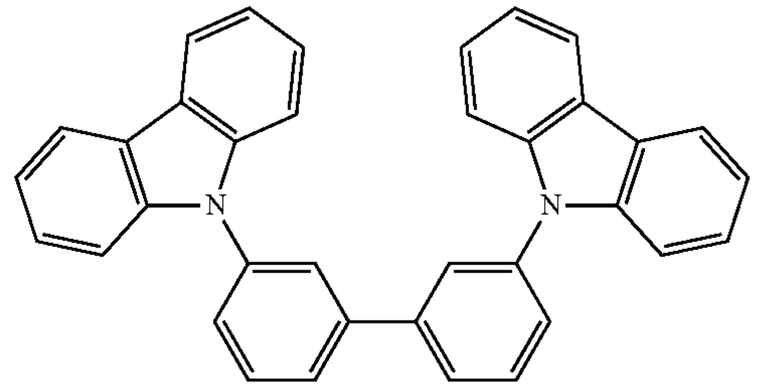
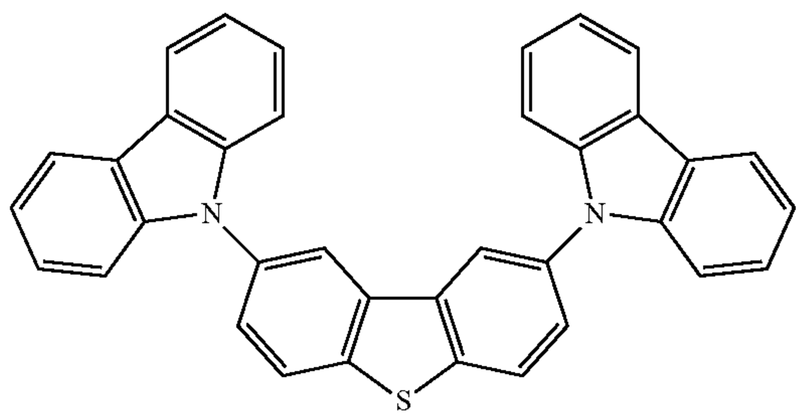
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal coordination complexes (e.g., Zn, Al with N^N ligands)		US20040137268, US20040137267
	Blue hosts	
Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
		US20070190359
Dibenzothiophene/ Dibenzofuran-carbazole compounds		WO2006114966, US20090167162

TABLE 1-continued

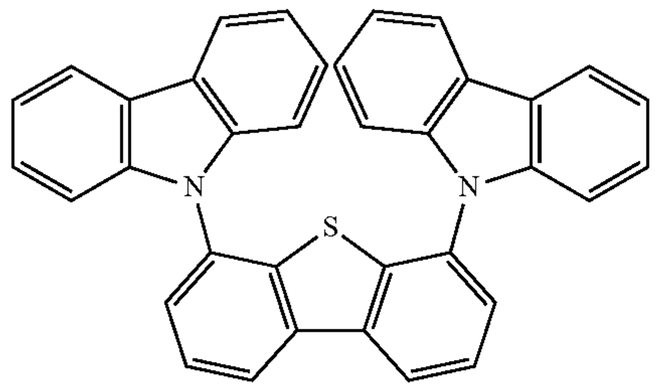
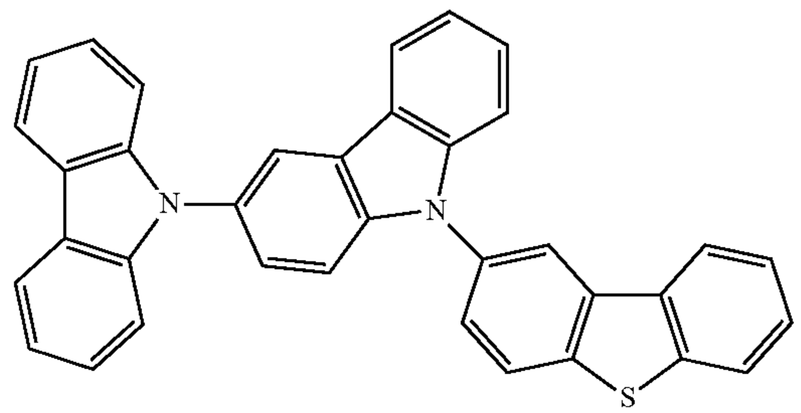
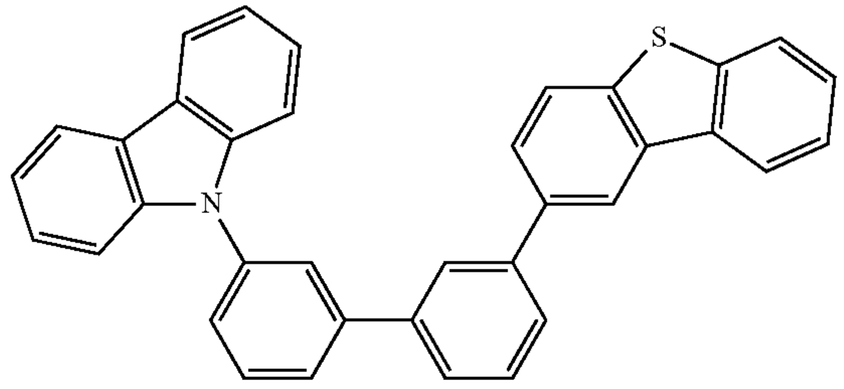
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090167162
		WO2009086028
		US20090030202, US20090017330

TABLE 1-continued

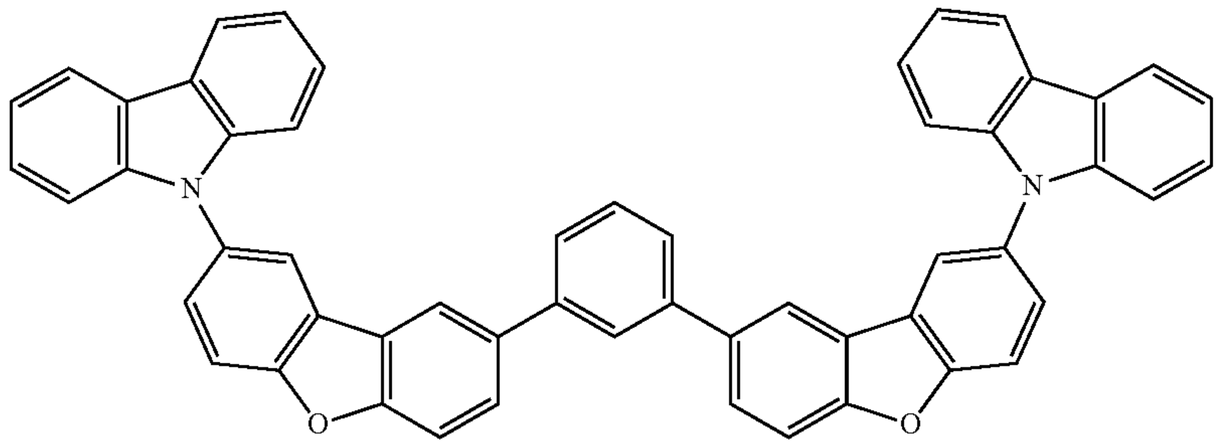
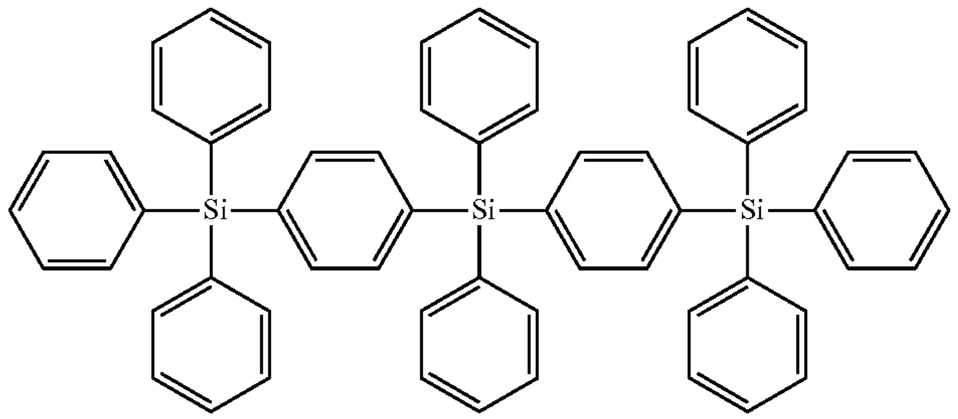
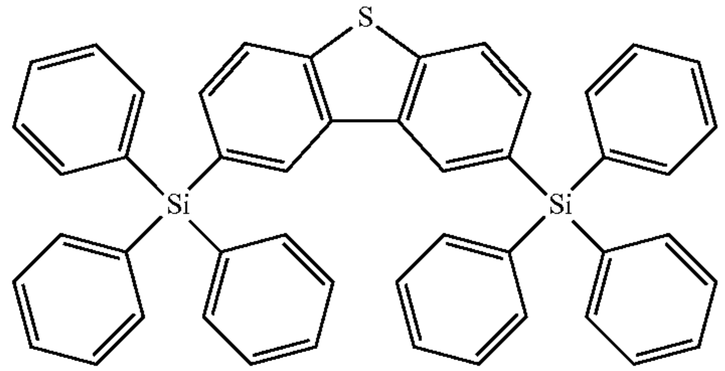
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20100084966
Silicon aryl compounds		US20050238919
		WO2009003898

TABLE 1-continued

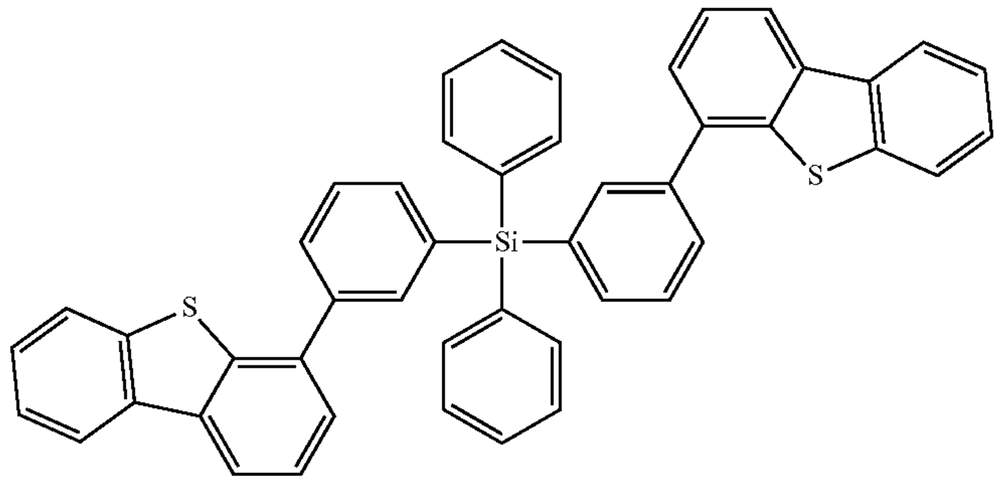
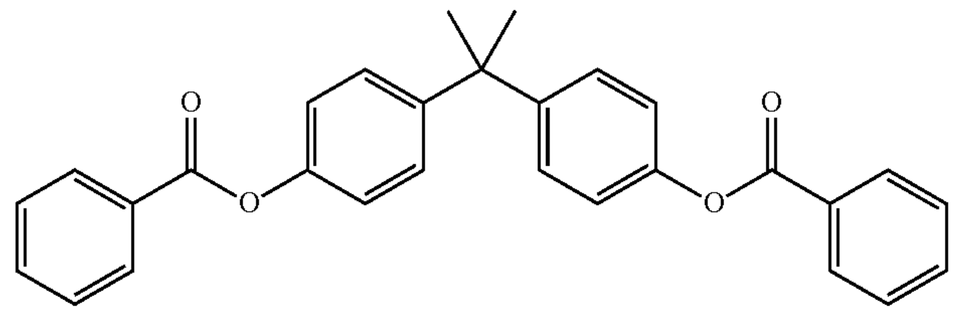
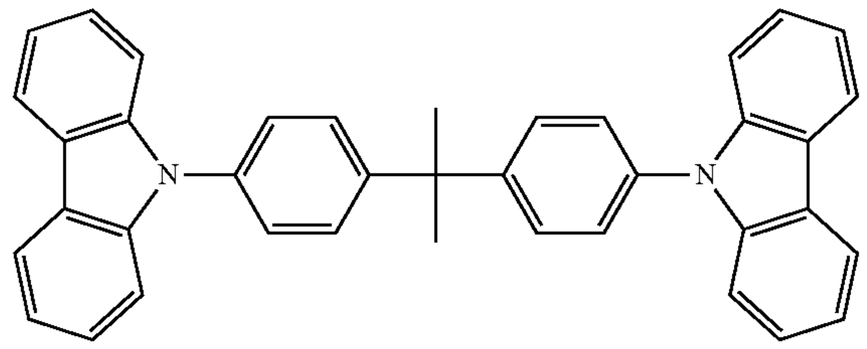
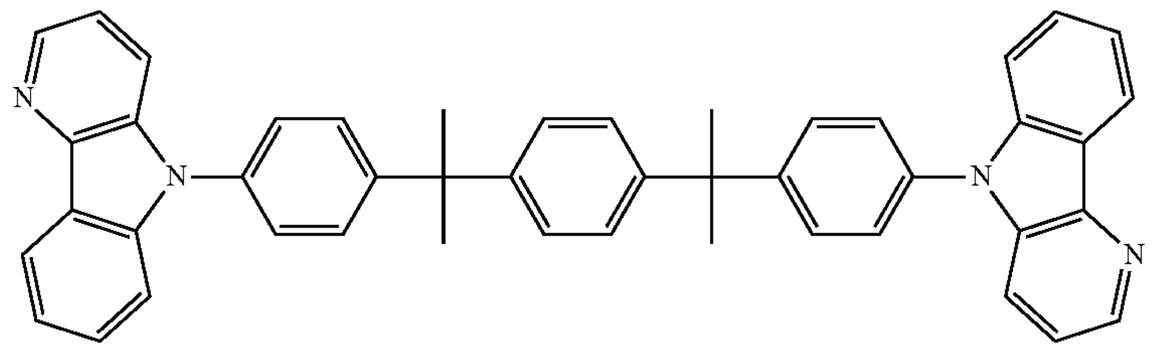
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silicon/ Germanium aryl compounds		EP2034538A
Aryl benzoyl ester		WO2006100298
Carbazole linked by non-conjugated groups		US20040115476
Aza-carbazoles		US20060121308

TABLE 1-continued

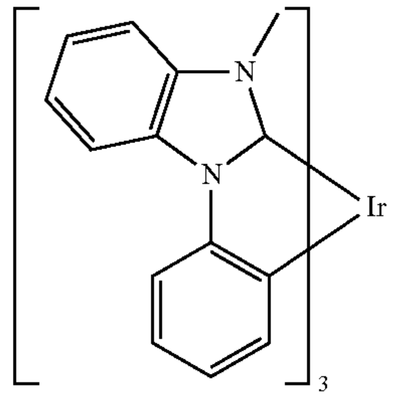
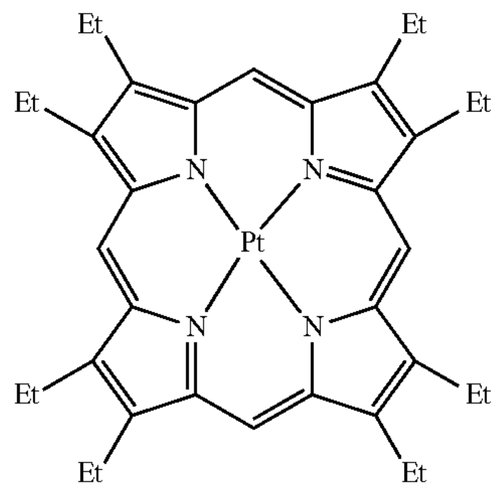
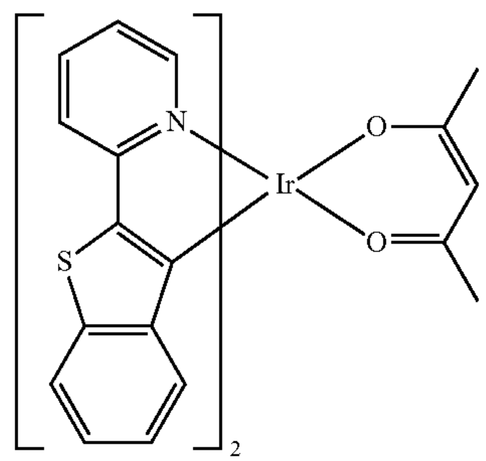
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
High triplet metal organo-metallic complex		US7154114
	Phosphorescent dopants Red dopants	
Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)

TABLE 1-continued

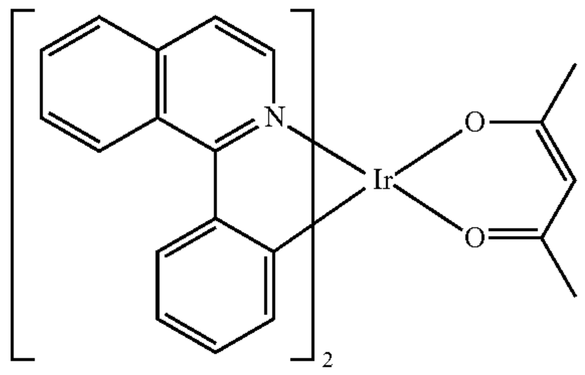
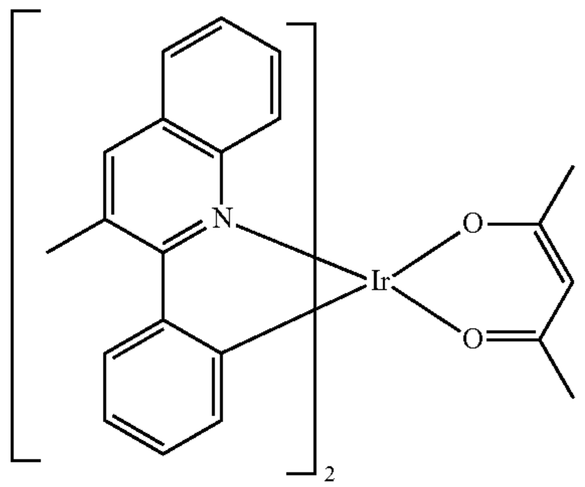
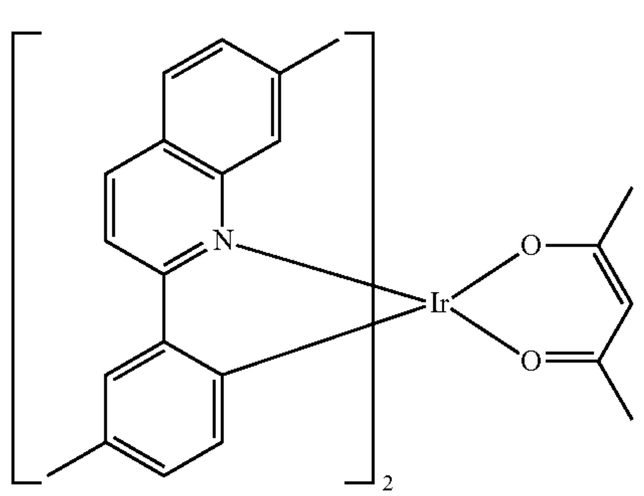
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US2006835469
		US2006835469
		US20060202194

TABLE 1-continued

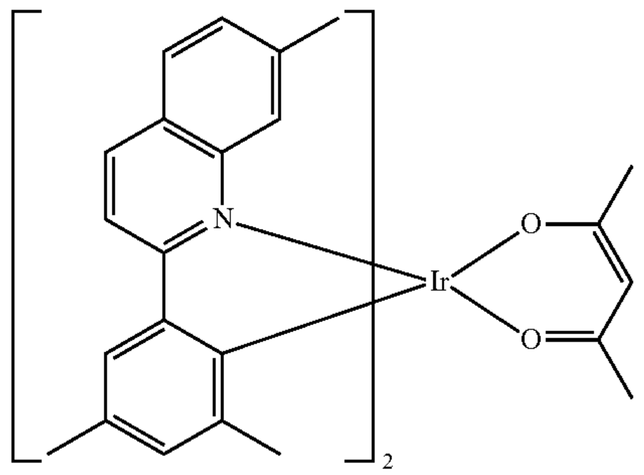
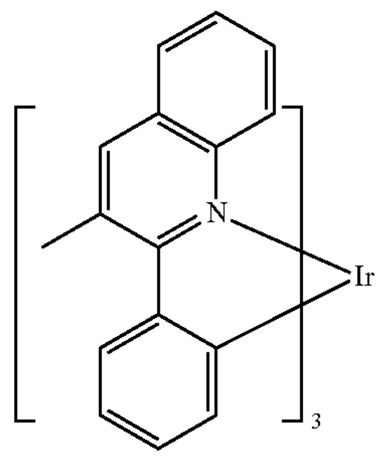
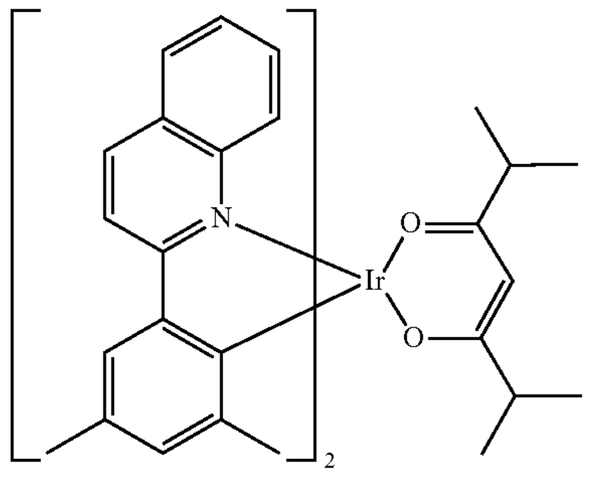
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060202194
		US20070087321
		US20080261076 US20100090591

TABLE 1-continued

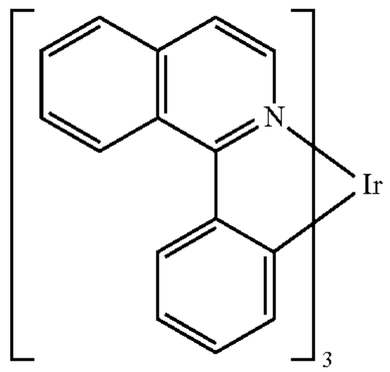
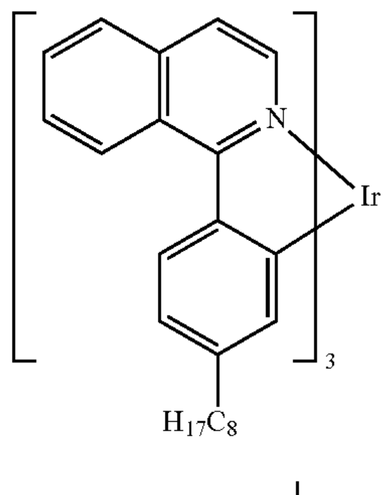
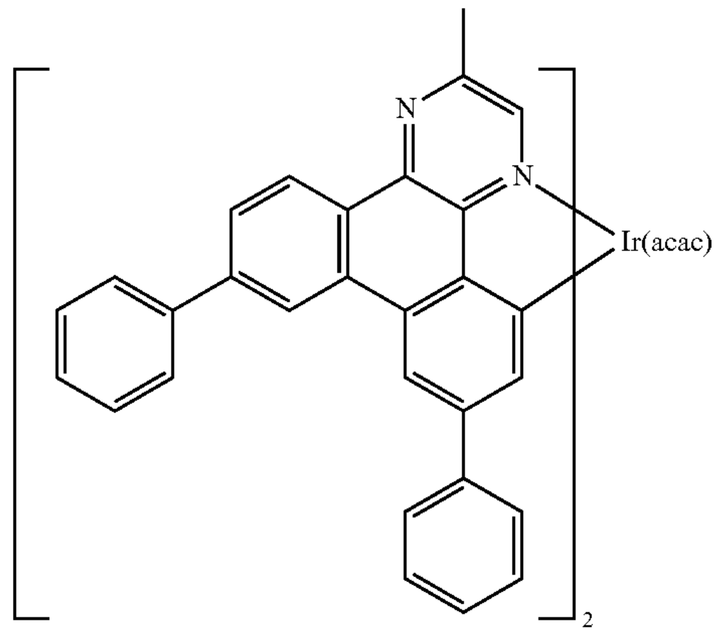
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070087321
		Adv. Mater. 19, 739 (2007)
		WO2009100991

TABLE 1-continued

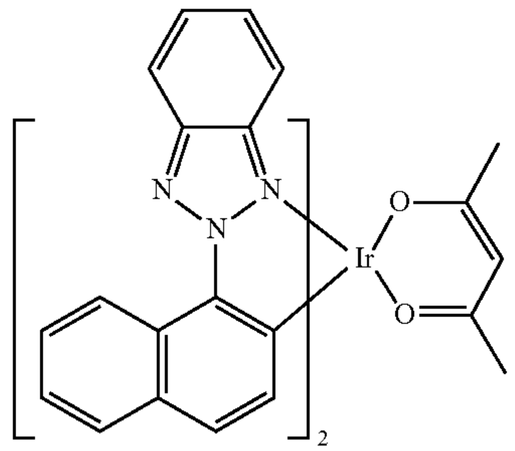
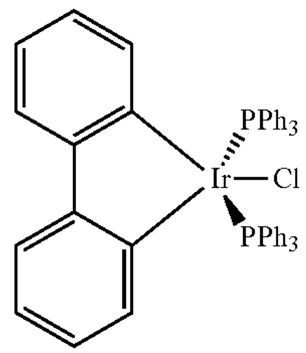
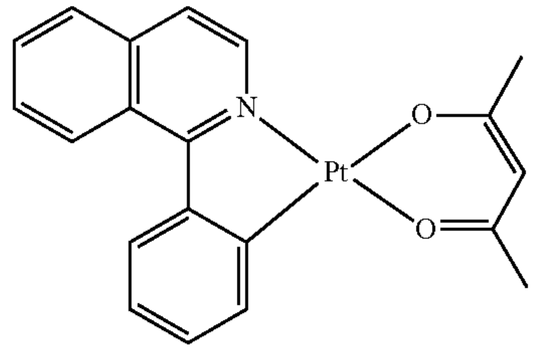
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2008101842
		US7232618
Platinum(II) organometallic complexes		WO2003040257

TABLE 1-continued

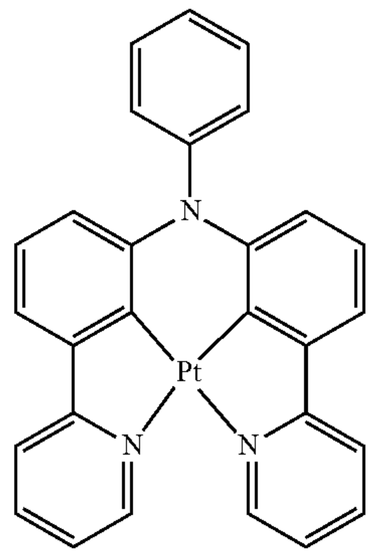
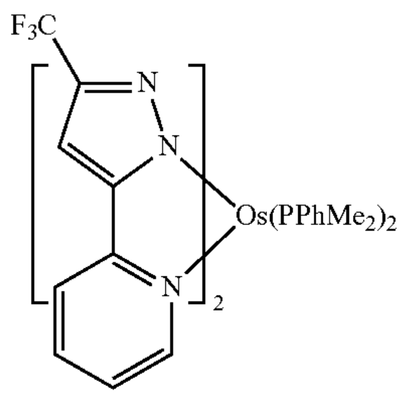
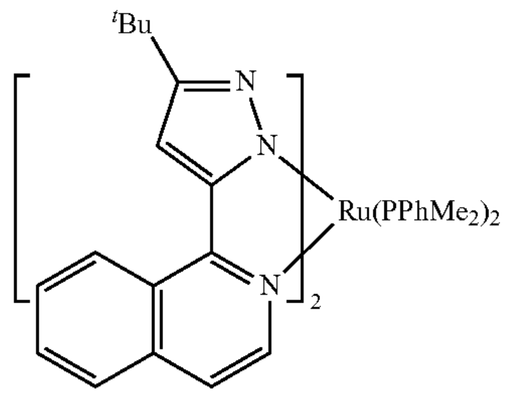
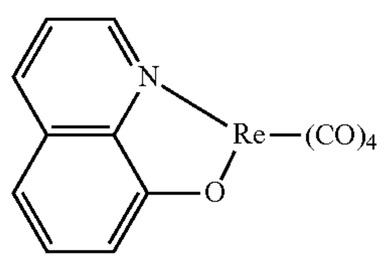
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070103060
Osminum(III) complexes		Chem. Mater. 17, 3532 (2005)
Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
Rhenium (I), (II), and (III) complexes		US20050244673

TABLE 1-continued

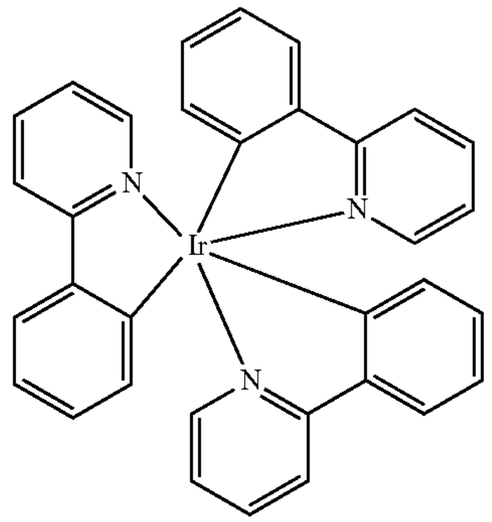
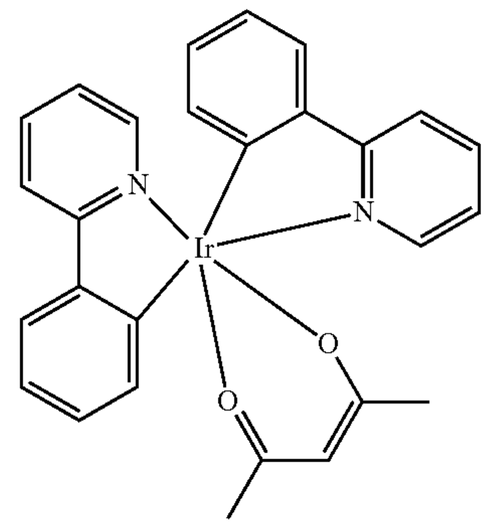
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	Green dopants	
Iridium(III) organometallic complexes	 and its derivatives	Inorg. Chem. 40, 1704 (2001)
		US20020034656

TABLE 1-continued

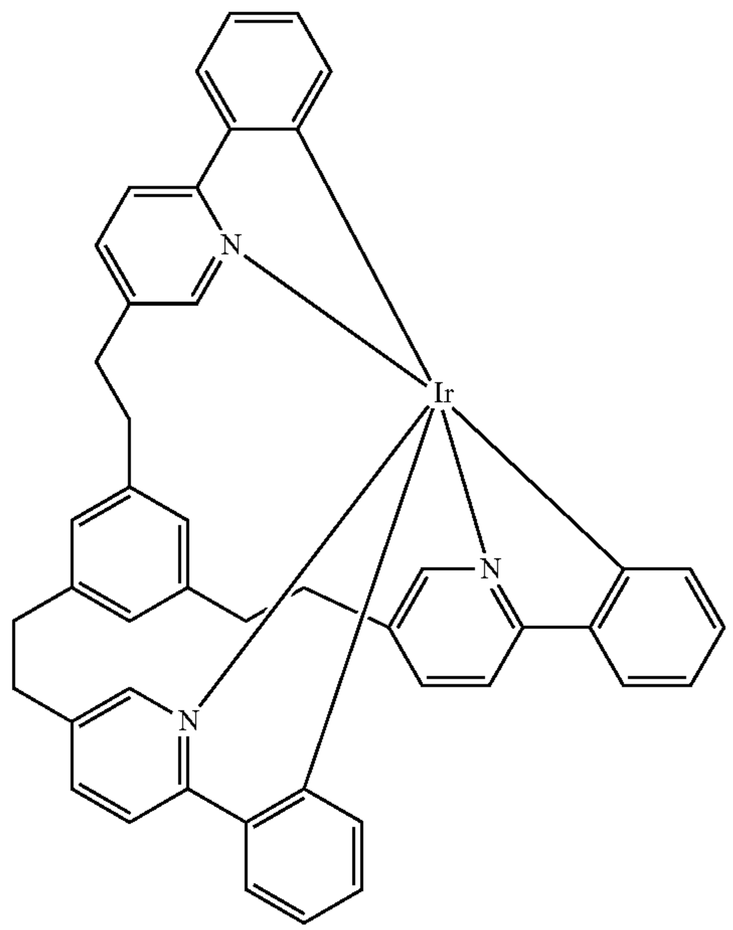
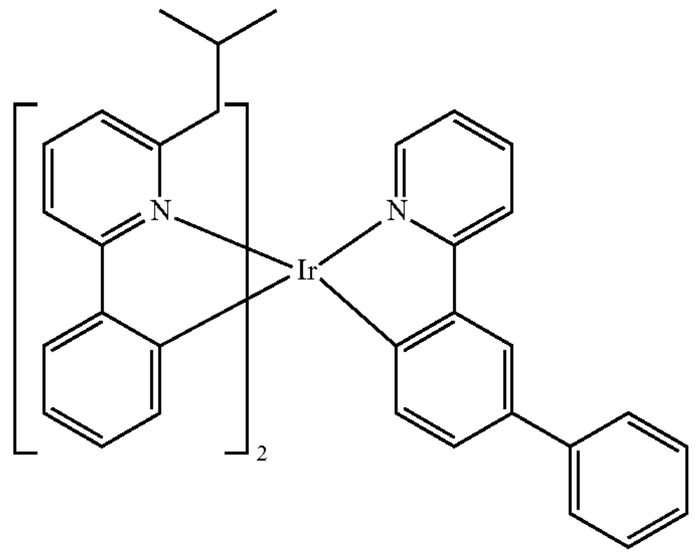
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7332232
		US20090108737

TABLE 1-continued

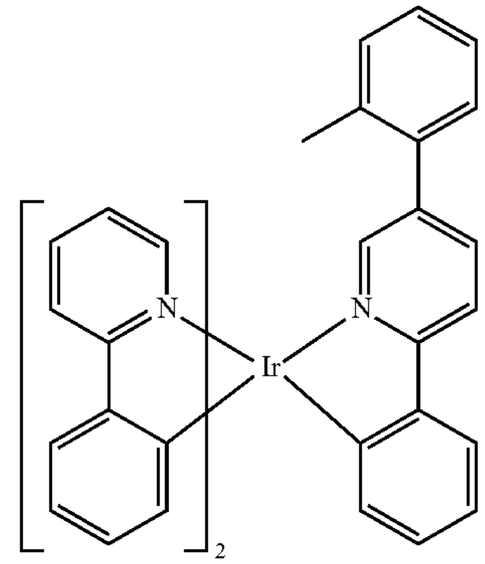
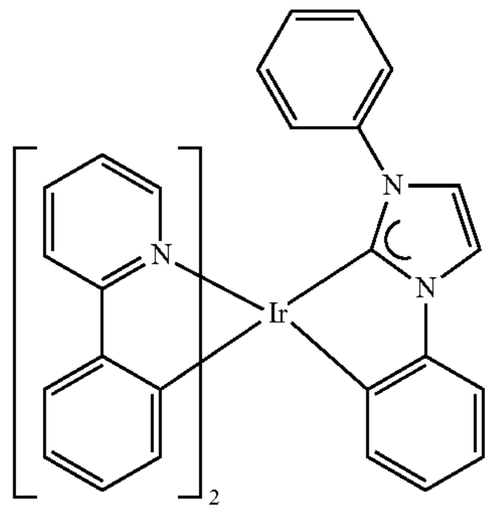
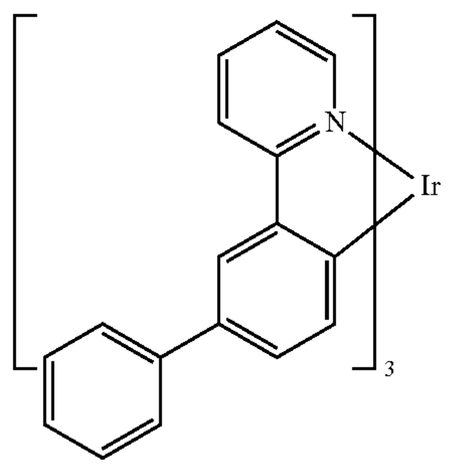
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2010028151
		EP1841834B
		US20060127696

TABLE 1-continued

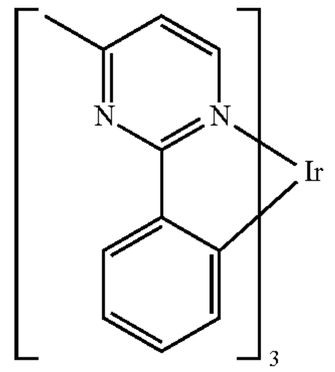
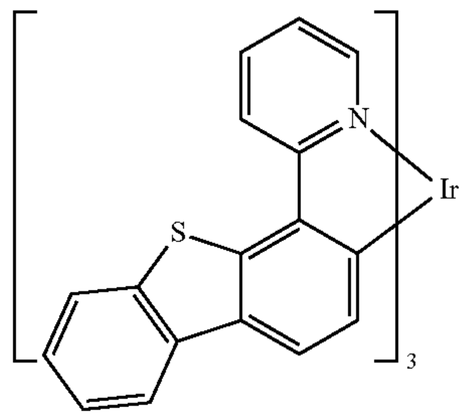
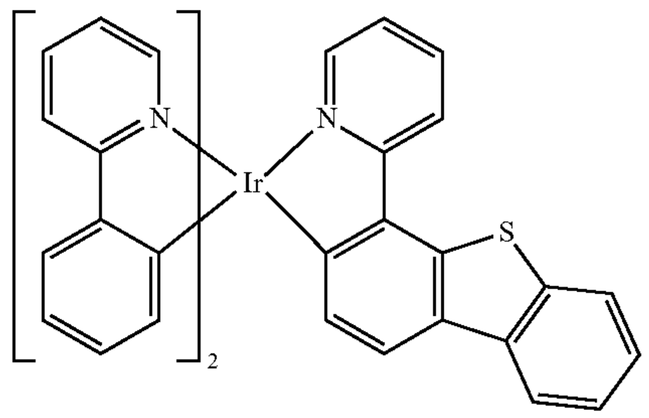
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090039776
		US6921915
		US20100244004

TABLE 1-continued

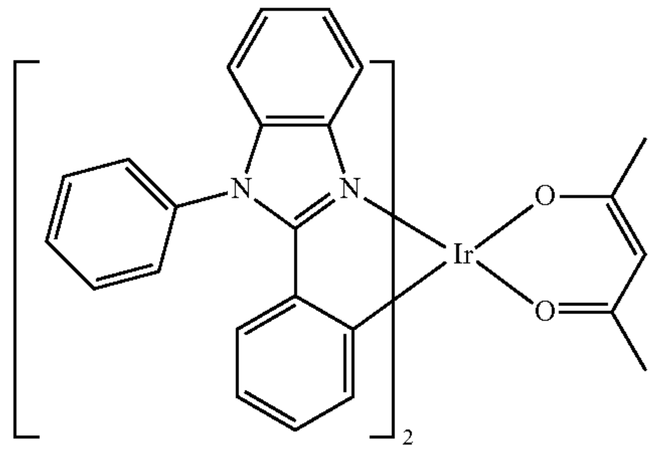
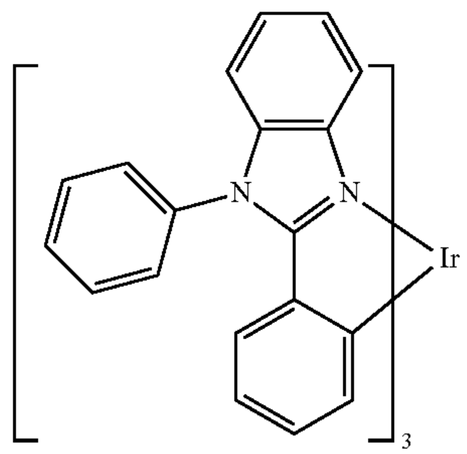
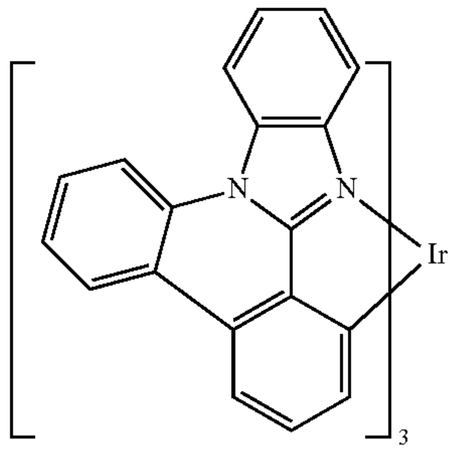
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US6687266
		Chem. Mater. 16, 2480 (2004)
		US20070190359

TABLE 1-continued

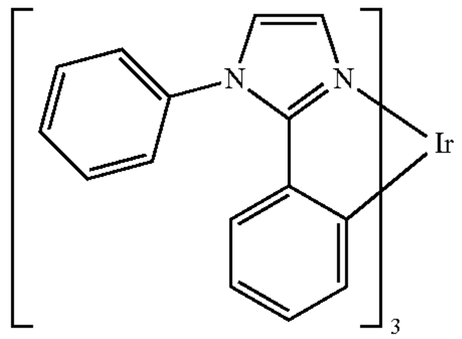
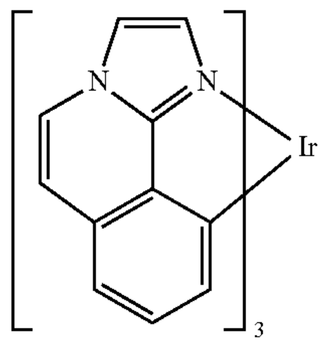
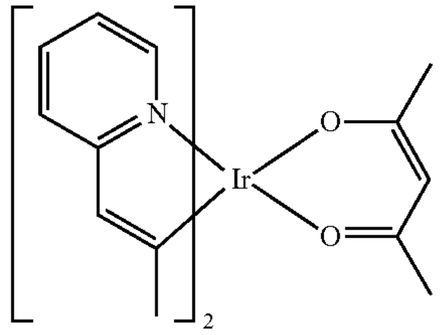
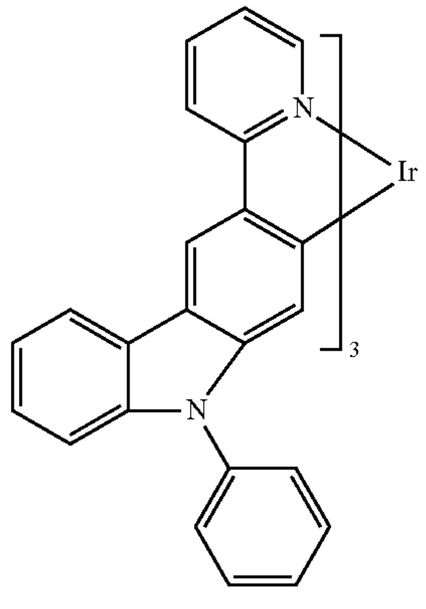
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US 20060008670 JP2007123392
		WO2010086089, WO2011044988
		Adv. Mater. 16, 2003 (2004)
		Angew. Chem. Int. Ed. 2006, 45, 7800

TABLE 1-continued

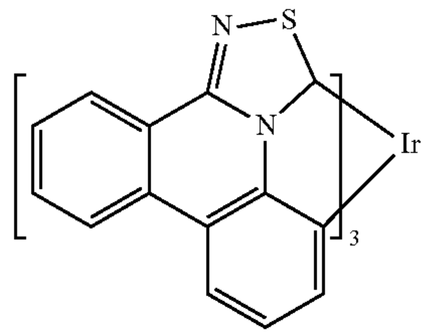
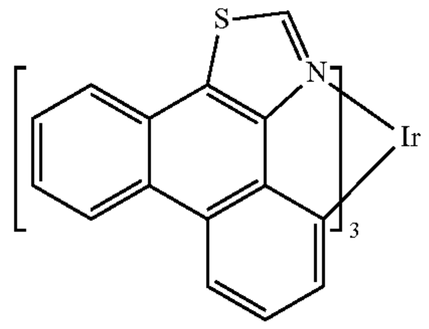
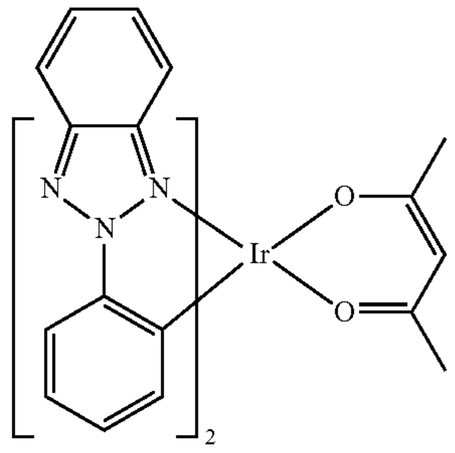
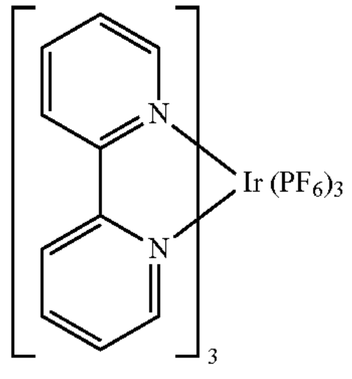
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009050290
		US20090165846
		US20080015355
		US20010015432

TABLE 1-continued

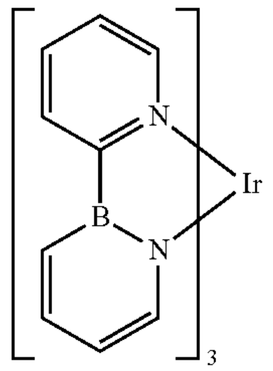
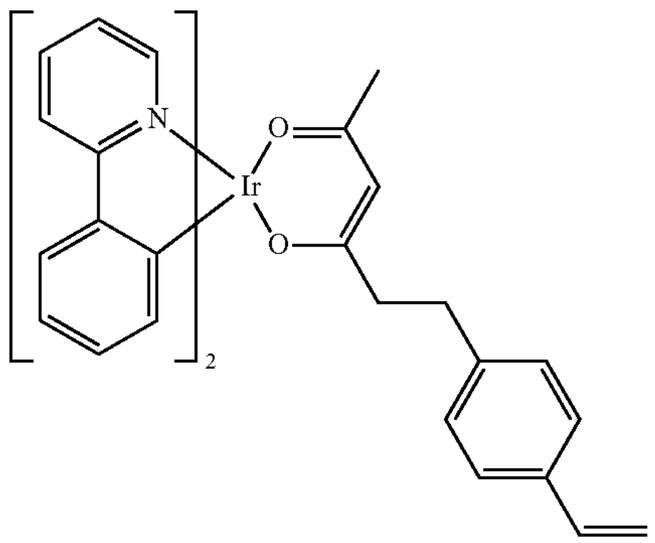
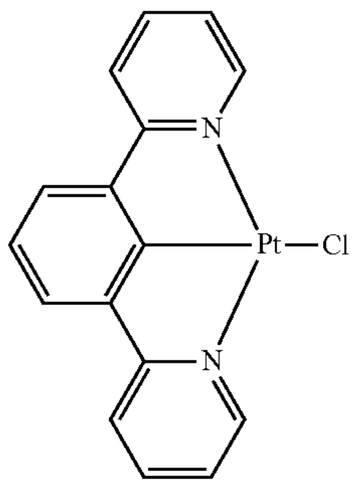
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20100295032
Monomer for polymeric metal organometallic compounds		US7250226, US7396598
Pt(II) organo-metallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)

TABLE 1-continued

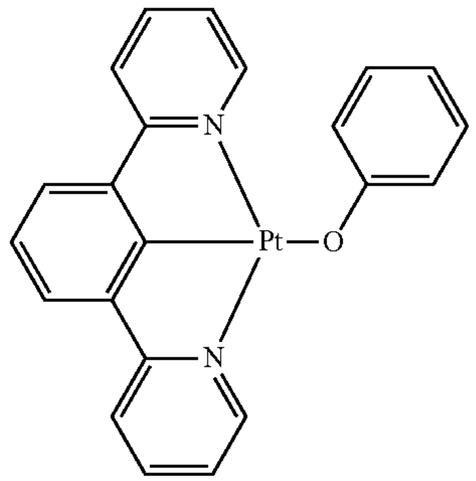
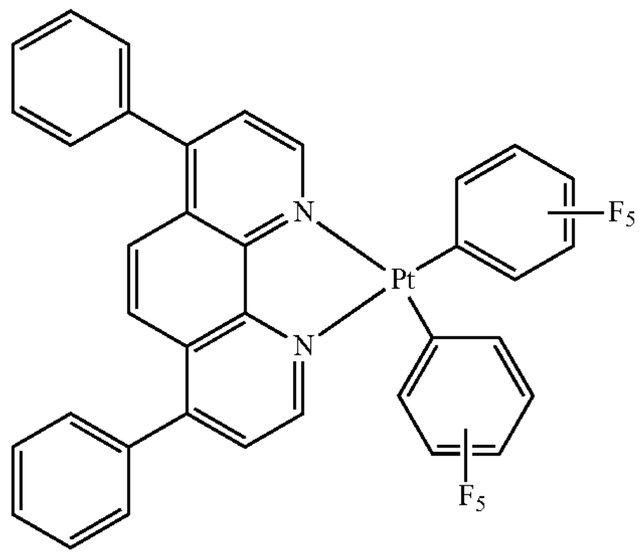
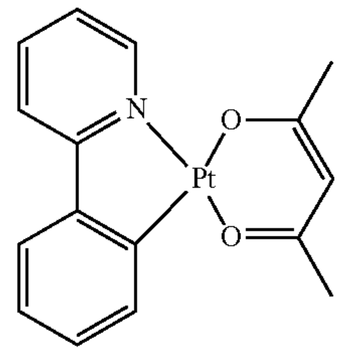
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645

TABLE 1-continued

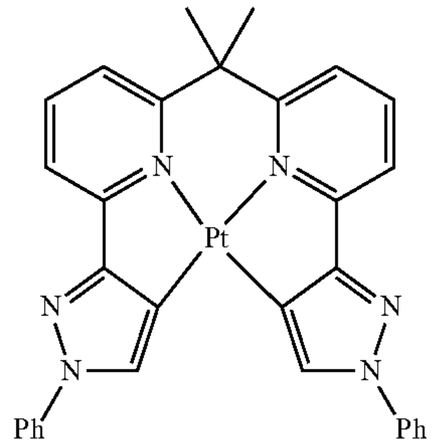
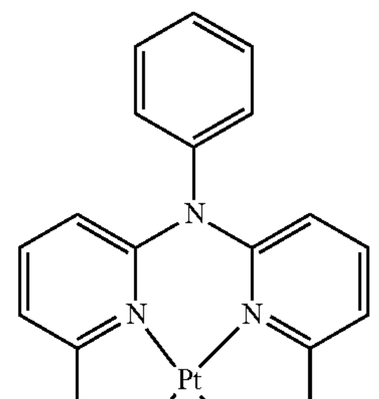
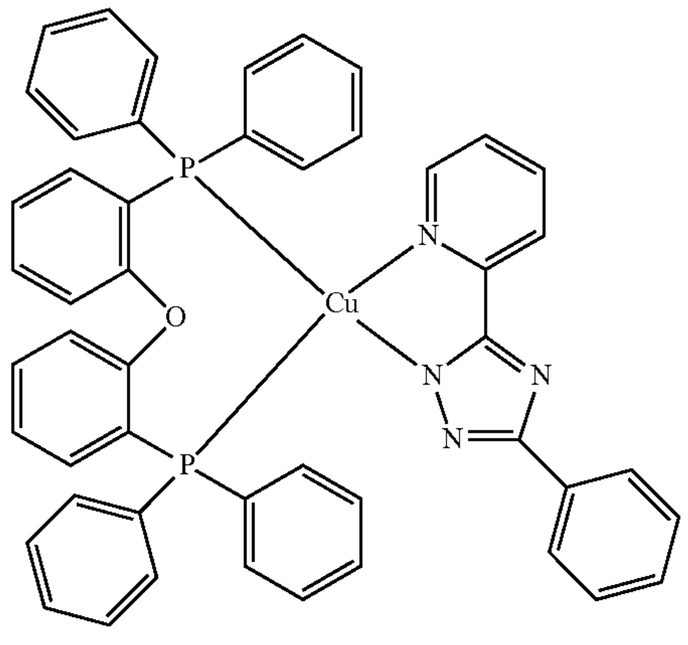
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060263635
		US20060182992 US20070103060
Cu complexes		WO2009000673

TABLE 1-continued

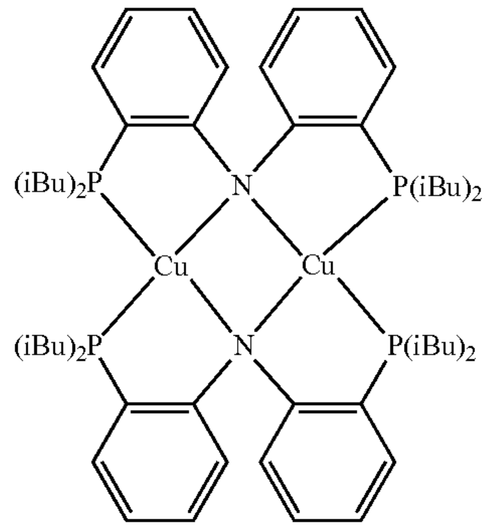
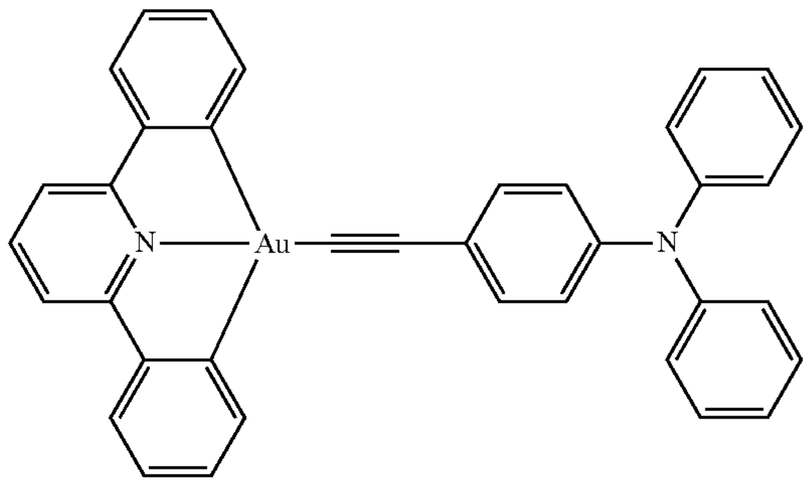
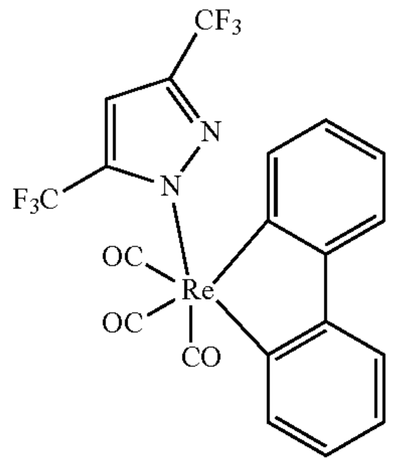
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070111026
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes		Inorg. Chem. 42, 1248 (2003)

TABLE 1-continued

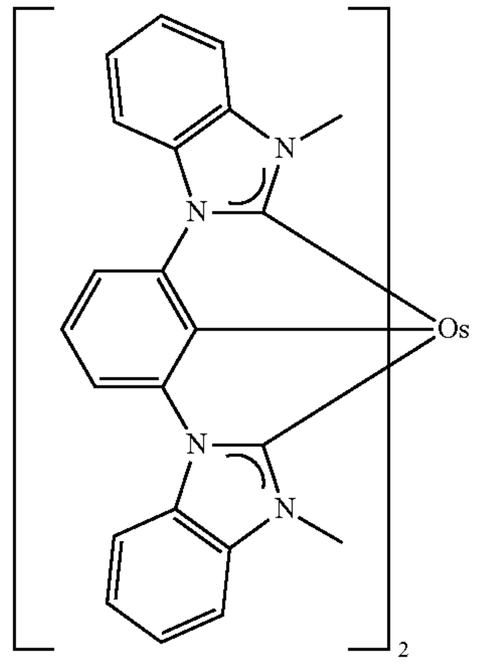
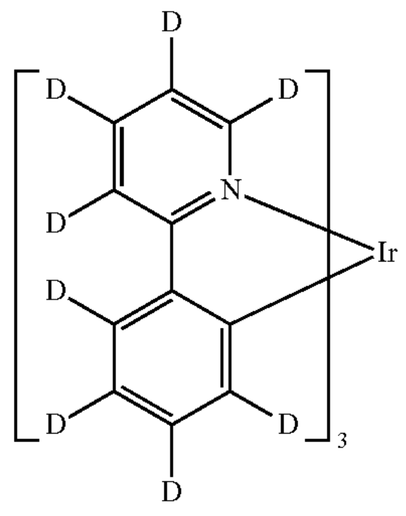
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Osmium(II) complexes		US7279704
Deuterated organometallic complexes		US20030138657

TABLE 1-continued

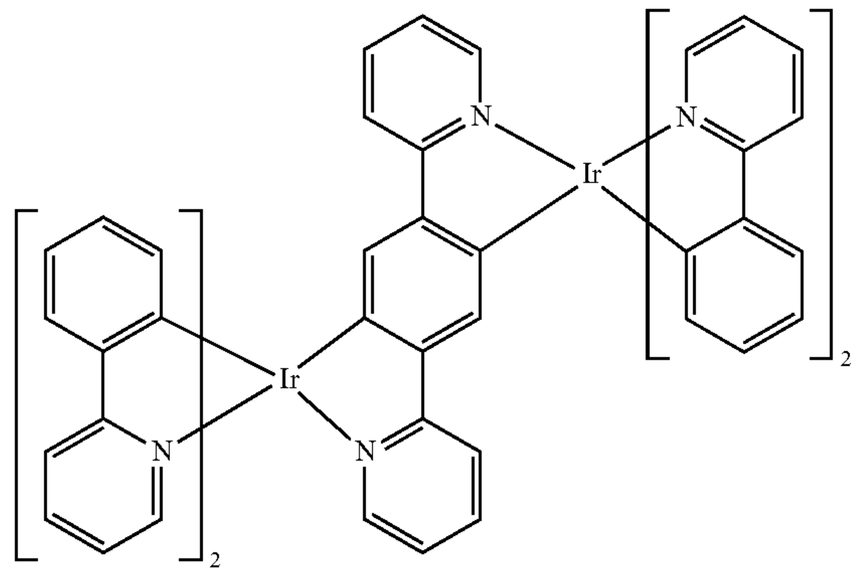
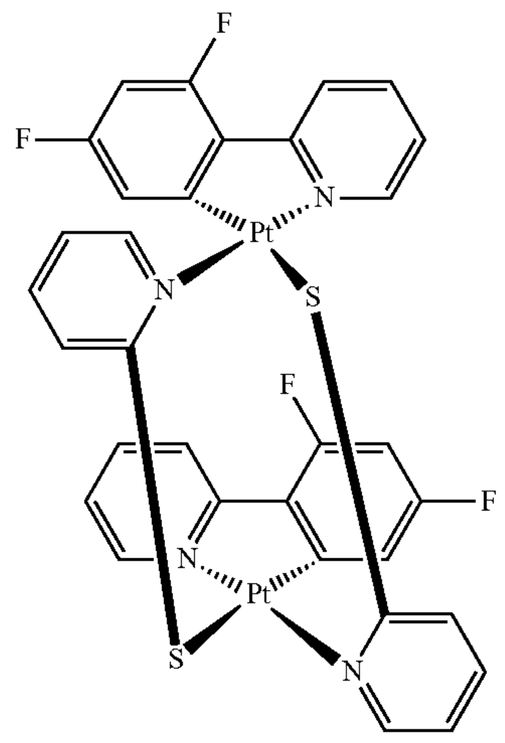
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Organometallic complexes with two or more metal centers		US20030152802
		US7090928
Blue dopants		

TABLE 1-continued

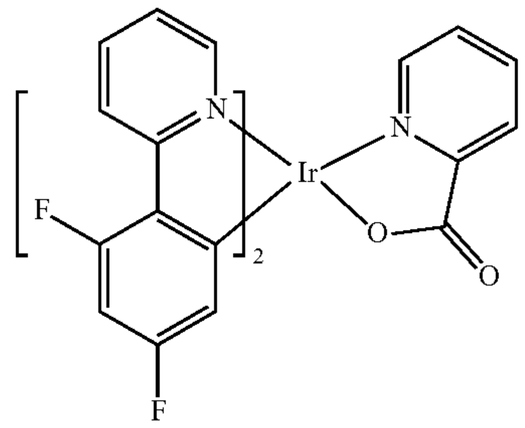
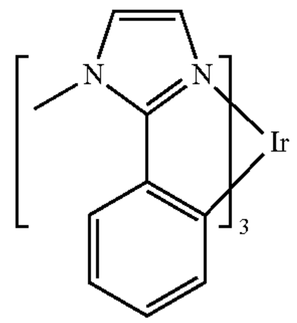
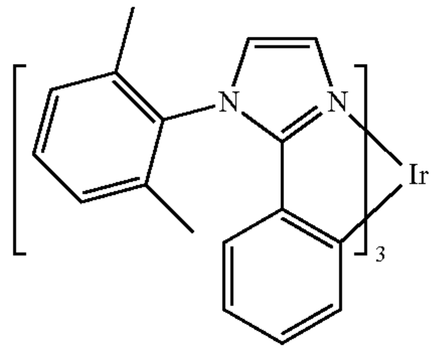
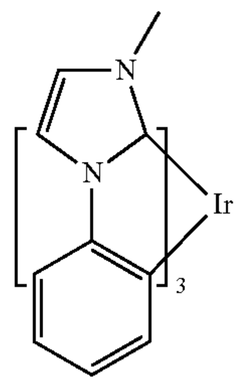
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		US7393599, WO2006056418, US20050260441, WO2005019373

TABLE 1-continued

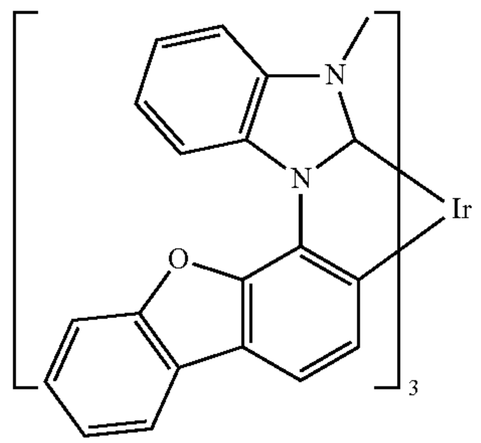
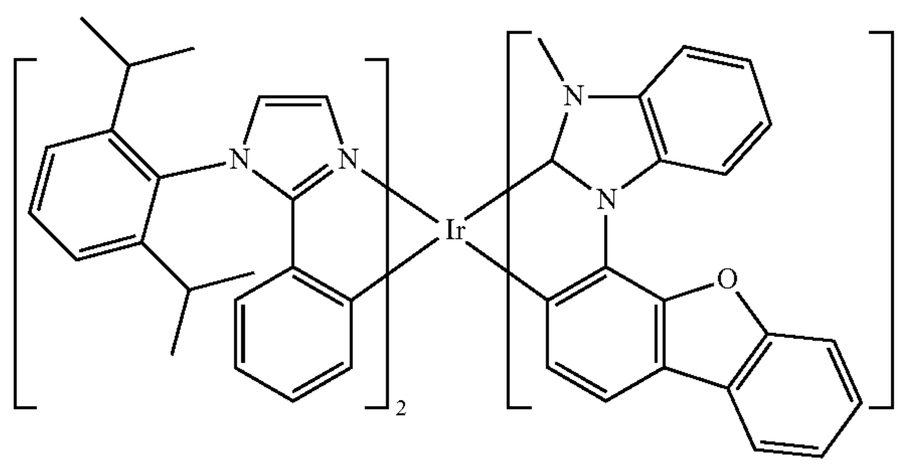
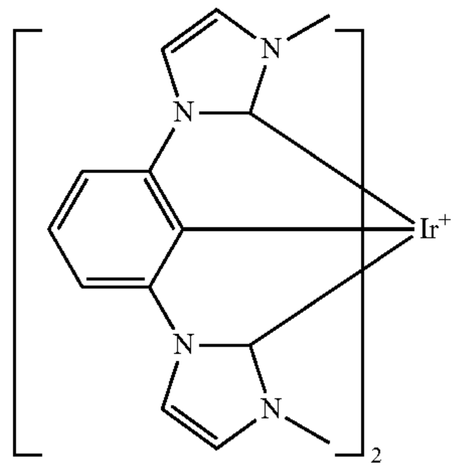
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US7534505
		WO2011051404
		US7445855

TABLE 1-continued

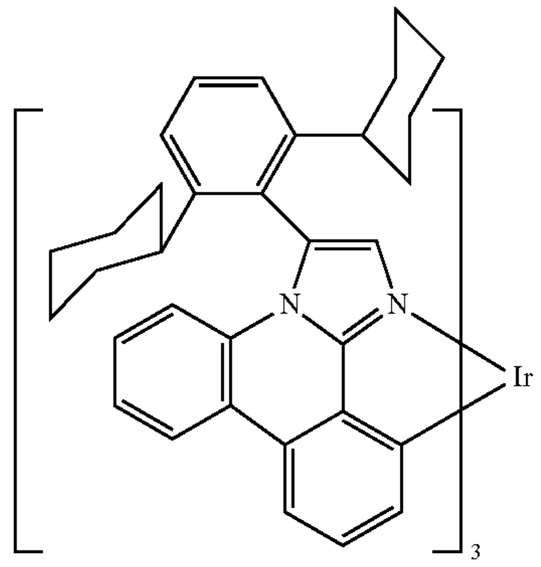
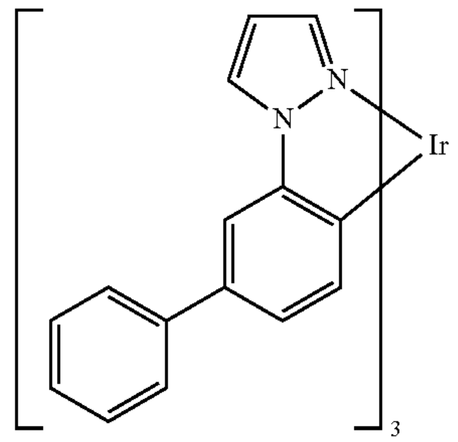
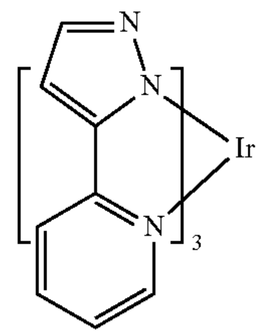
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20070190359, US20080297033 US20100148663
		US7338722
		US20020134984

TABLE 1-continued

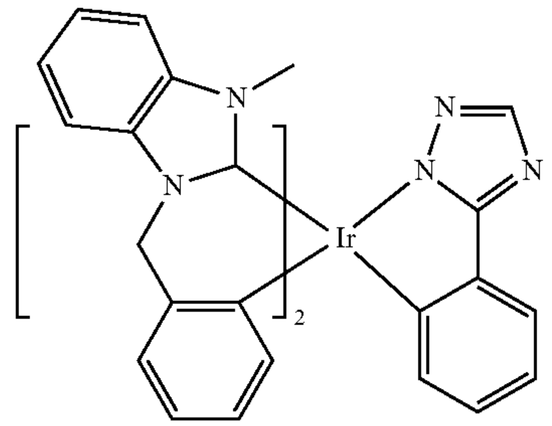
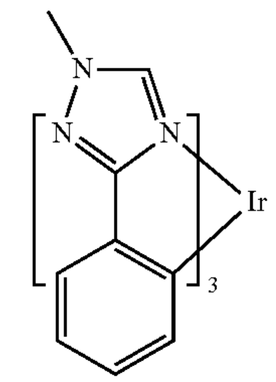
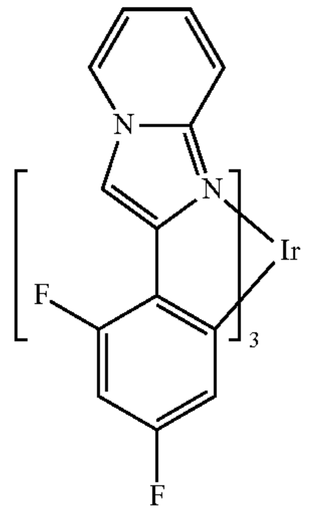
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Angew. Chem. Int. Ed. 47, 1 (2008)
		Chem. Mater. 18, 5119 (2006)
		Inorg. Chem. 46, 4308 (2007)

TABLE 1-continued

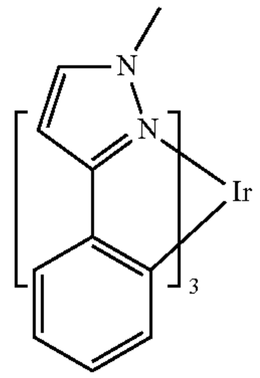
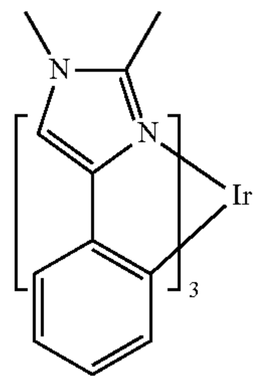
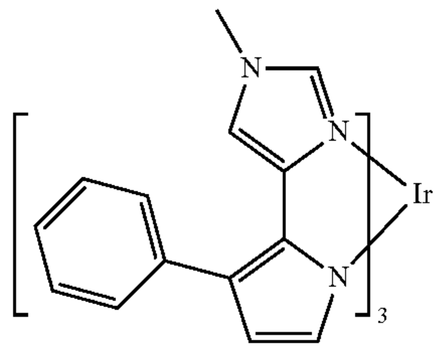
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2005123873
		WO2005123873
		WO2007004380

TABLE 1-continued

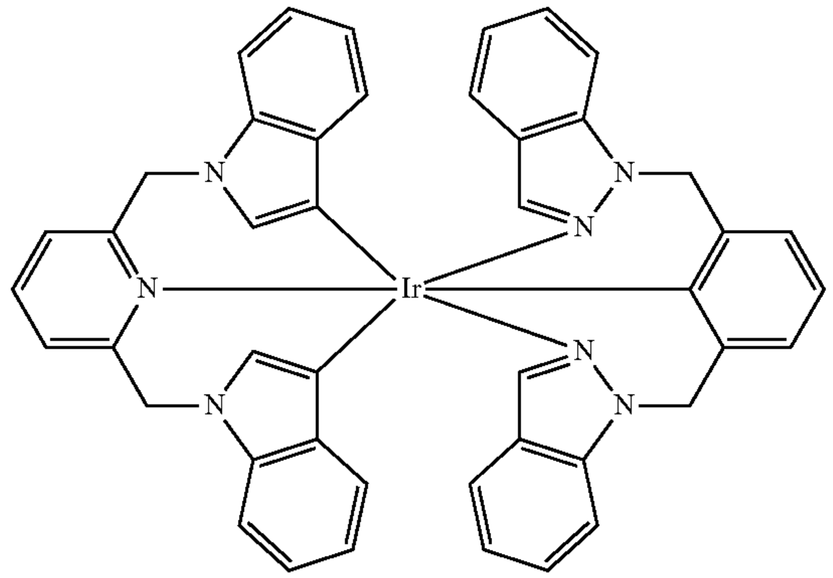
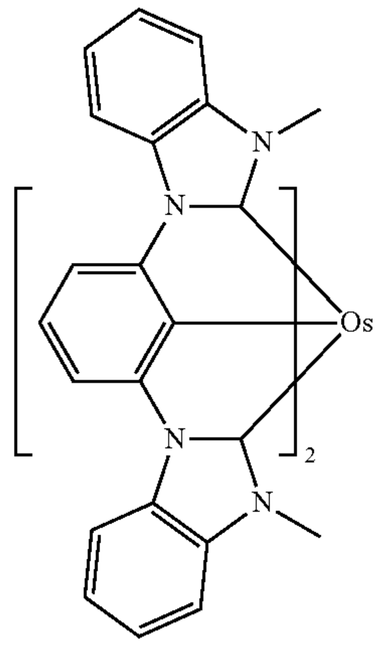
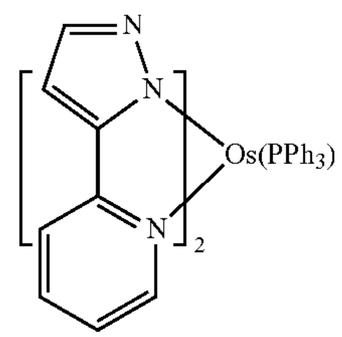
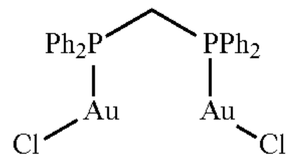
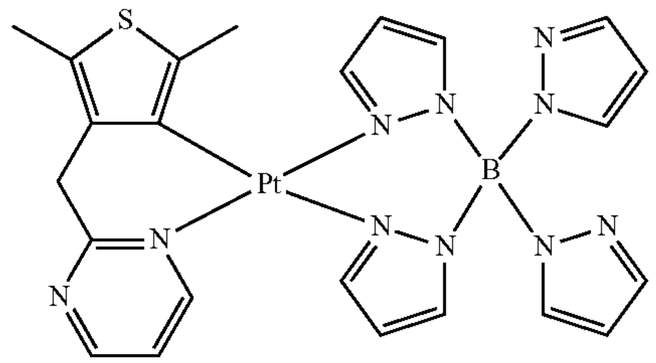
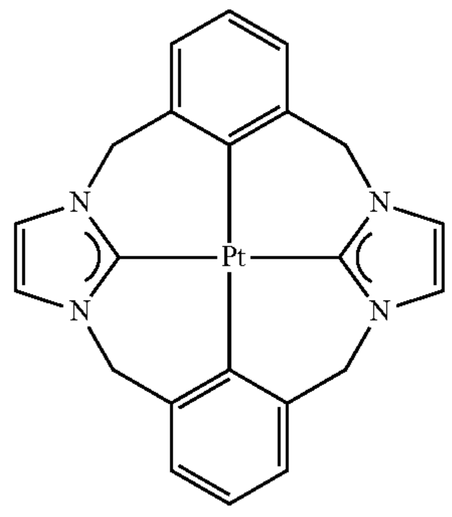
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2006082742
Osmium(II) complexes		US7279704
		Organometallics 23, 3745 (2004)

TABLE 1-continued

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Gold complexes		Appl. Phys. Lett. 74, 1361 (1999)
Platinum(II) complexes		WO2006098120, WO2006103874
Pt tetradentate complexes with at least one metal-carbene bond		US7655323

Exciton/hole blocking layer materials

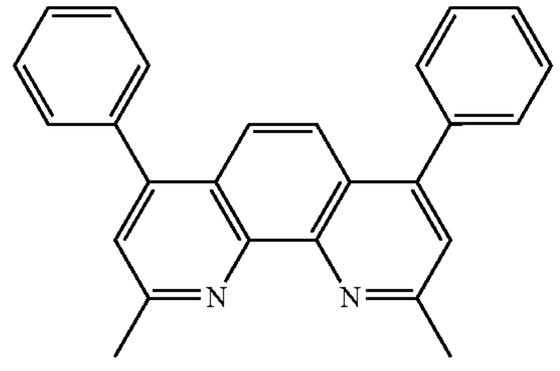
Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)

TABLE 1-continued

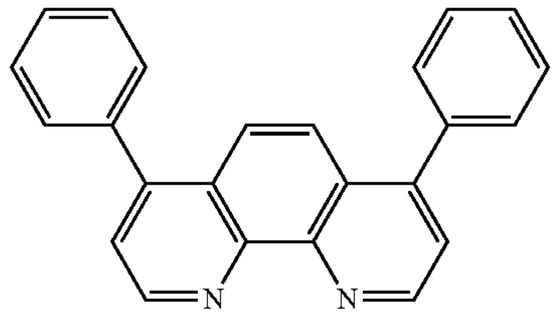
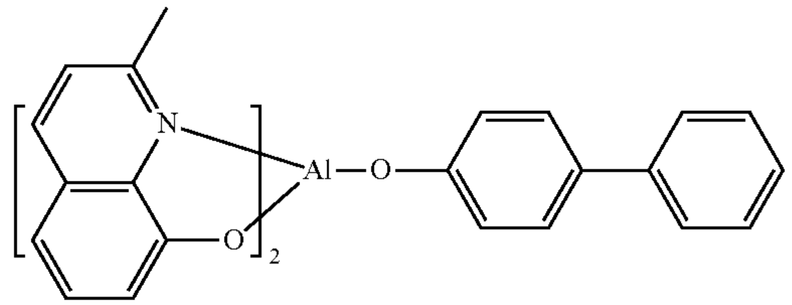
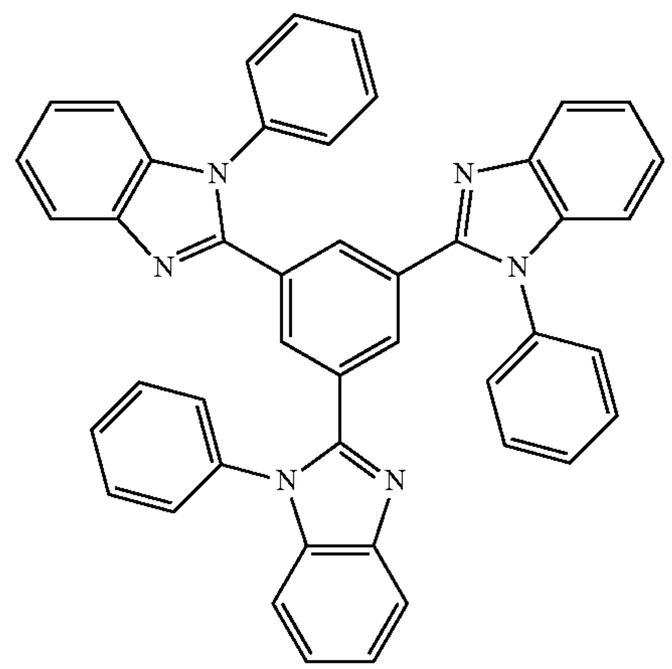
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		Appl. Phys. Lett. 79, 449 (2001)
Metal 8-hydroxy-quinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzo-imidazole		Appl. Phys. Lett. 81, 162 (2002)

TABLE 1-continued

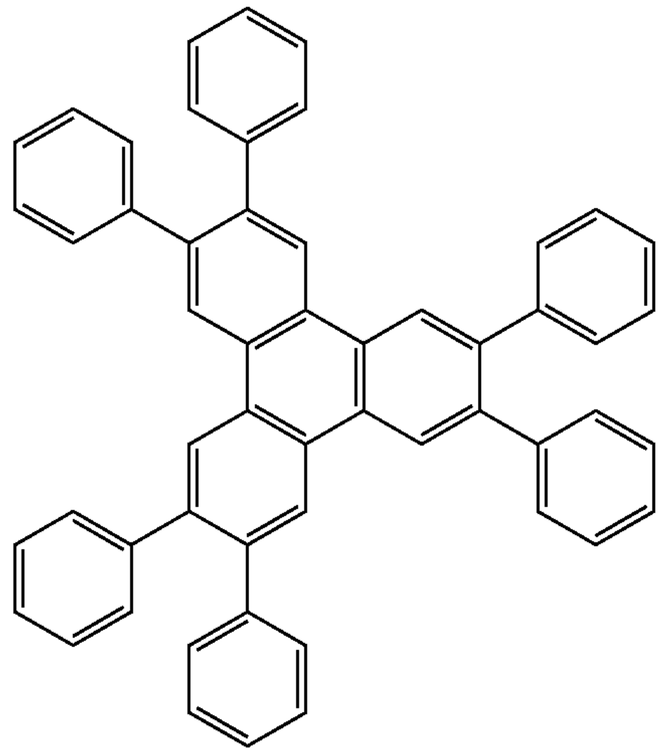
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triphenylene compounds		US20050025993

TABLE 1-continued

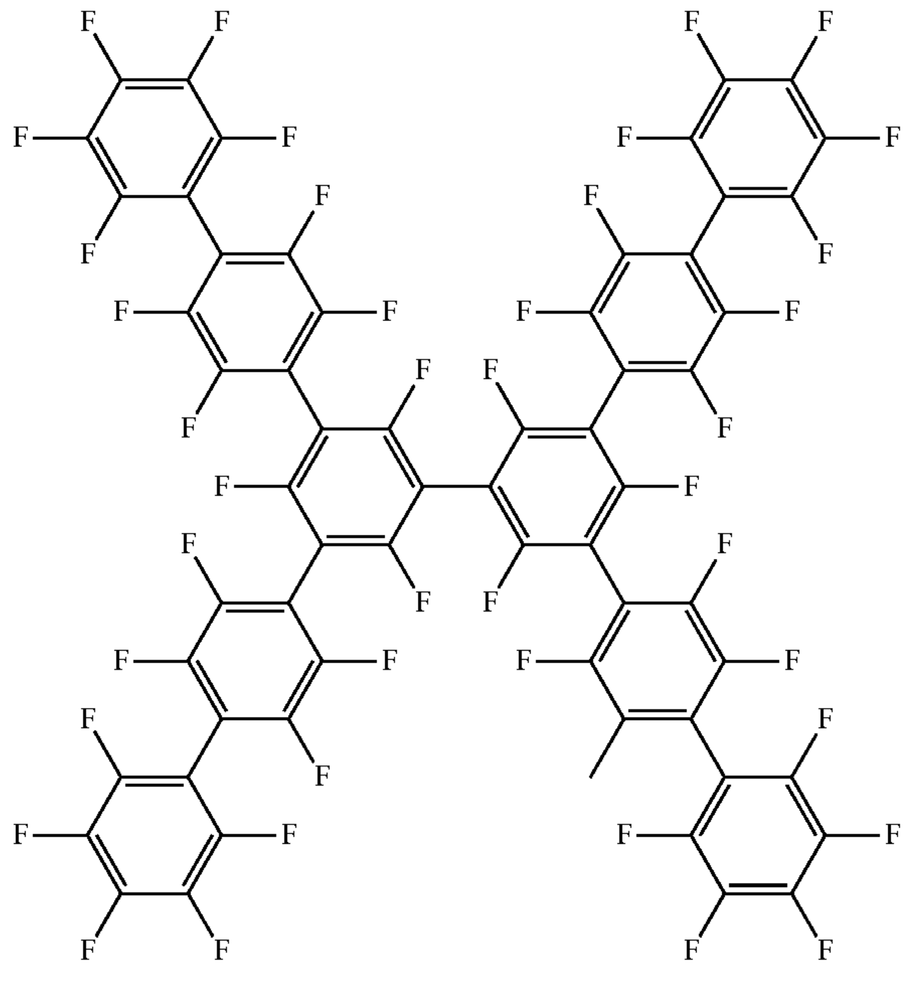
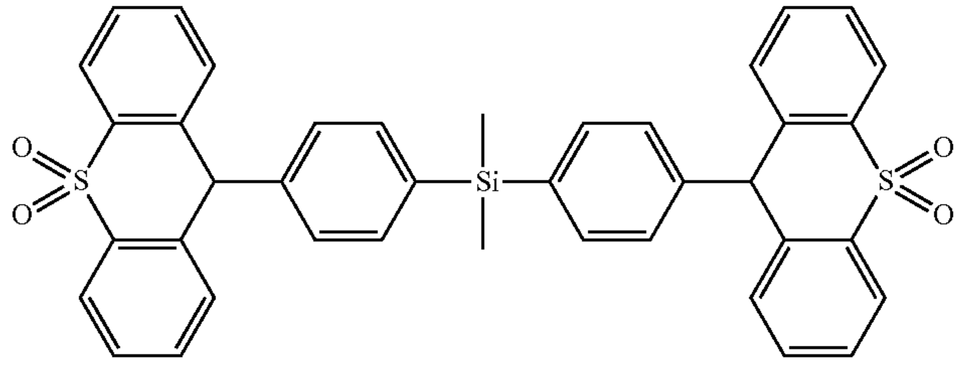
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Fluorinated aromatic compounds		Appl. Phys. Lett. 79, 156 (2001)
Phenothiazine-S-oxide		WO2008132085

TABLE 1-continued

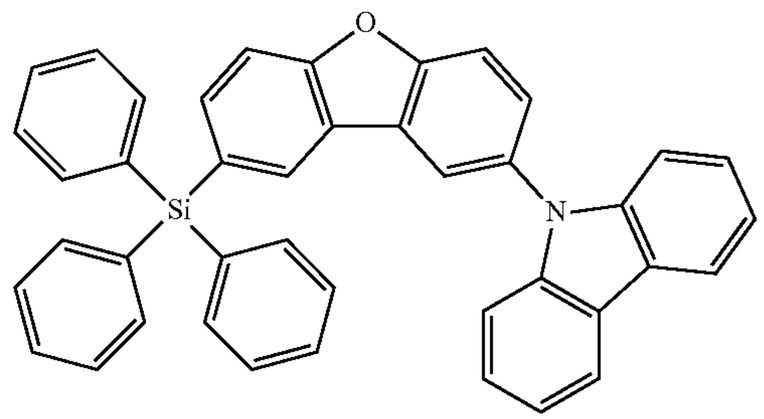
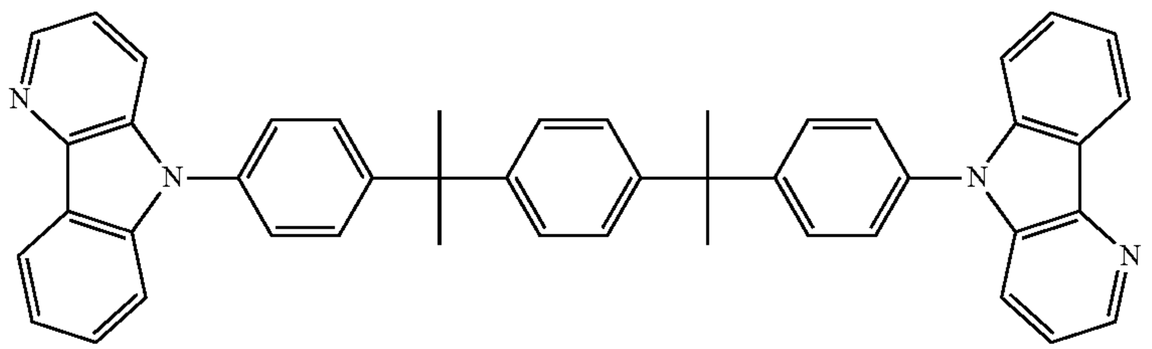
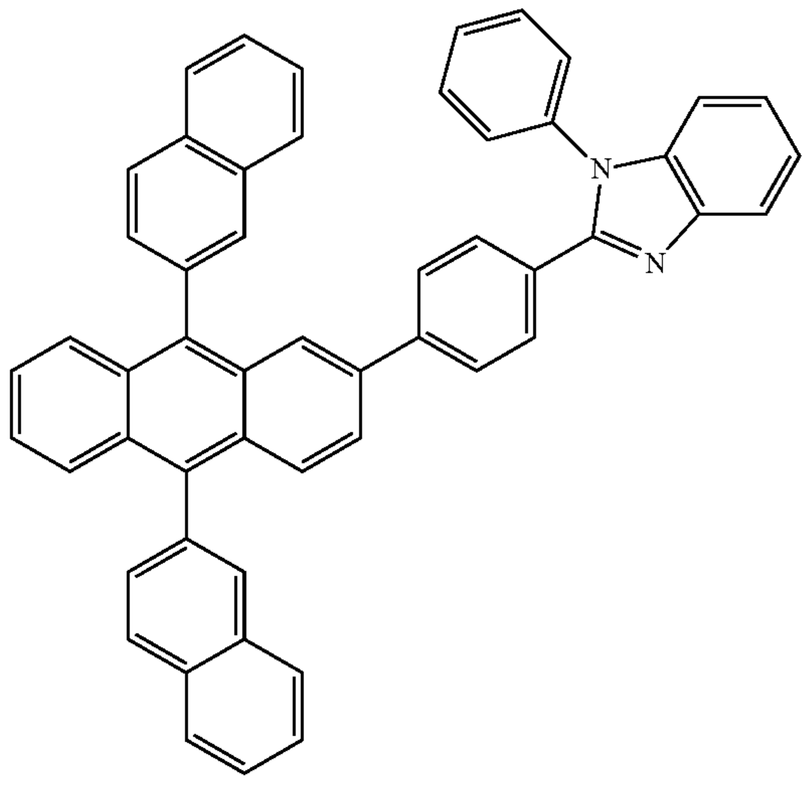
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzo-heterocycles		WO2010079051
Aza-carbazoles		US20060121308
Electron transporting materials		
Anthracene-benzoimidazole compounds		WO2003060956

TABLE 1-continued

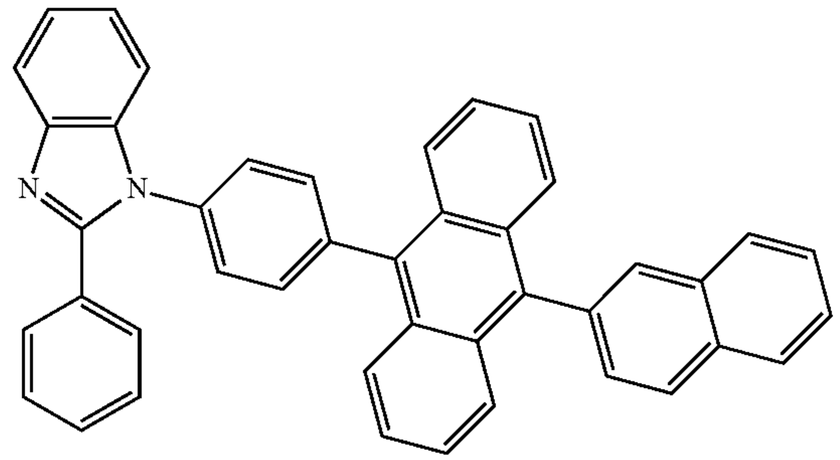
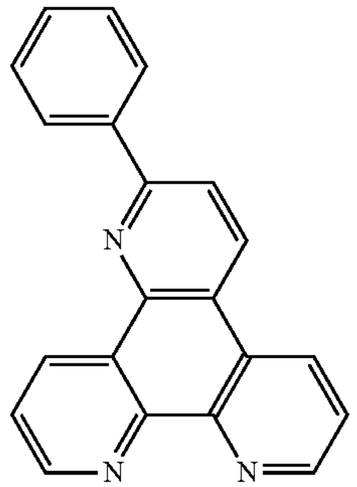
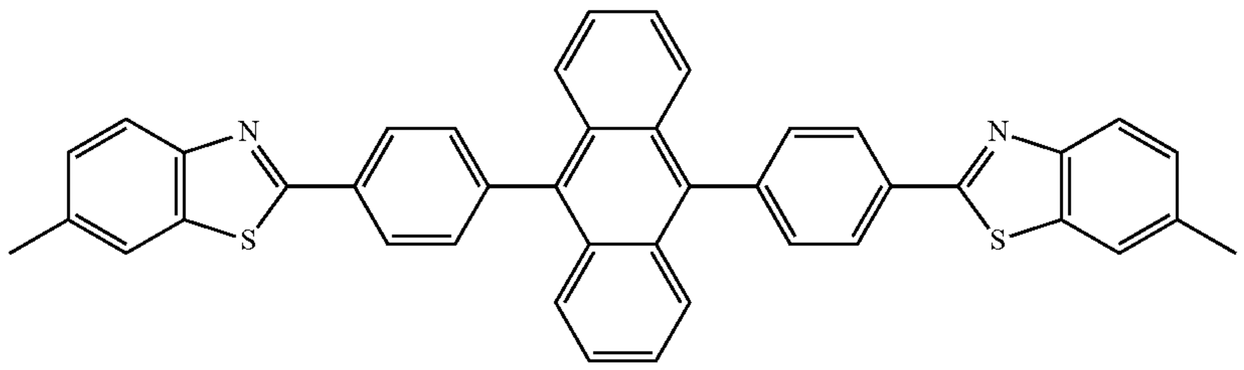
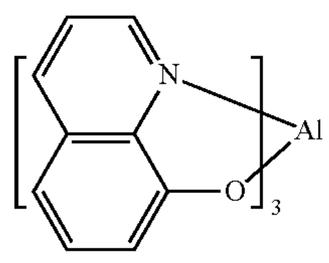
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20090179554
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxy-quinolates (e.g., Alq_3, Zrq_4)		Appl. Phys. Lett. 51, 913 (1987) US7230107

TABLE 1-continued

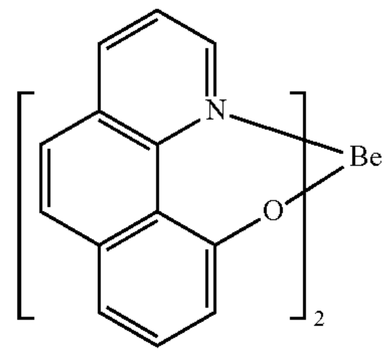
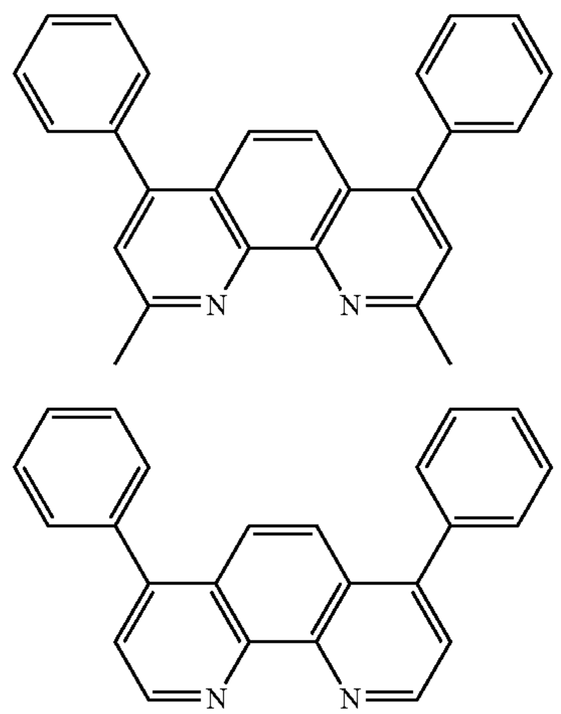
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal hydroxy-benoquinolates		Chem. Lett. 5, 905 (1993)
Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007) Appl. Phys. Lett. 79, 449 (2001)

TABLE 1-continued

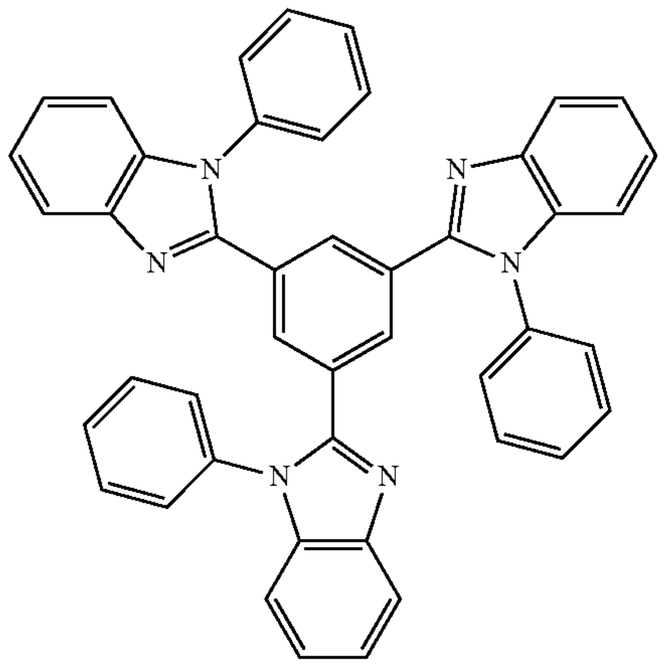
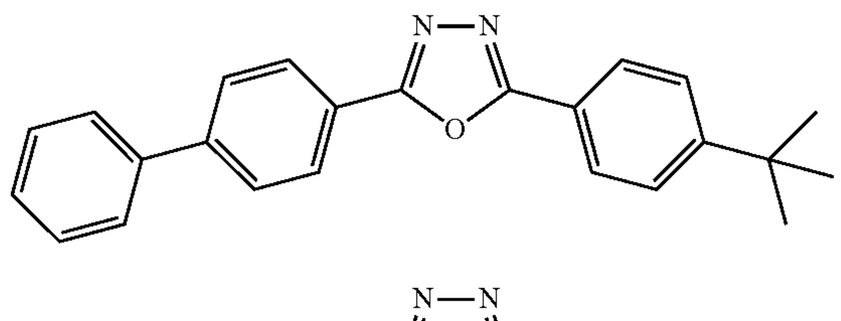
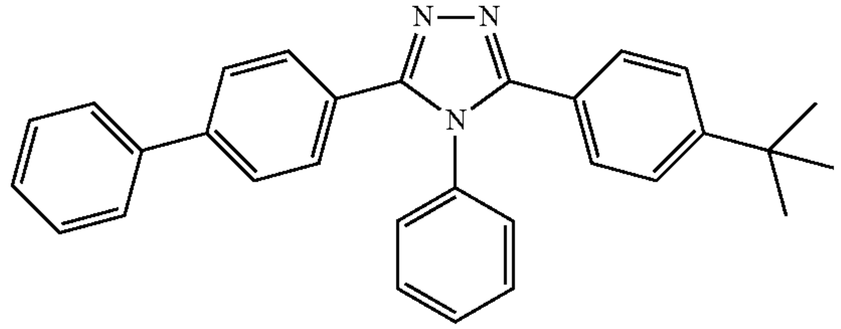
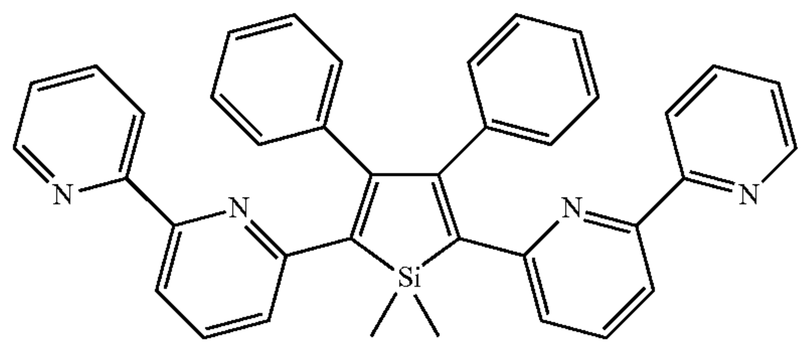
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
		Appl. Phys. Lett. 55, 1489 (1989)
		Jpn. J. Apply. Phys. 32, L917 (1993)
Silole compounds		Org. Electron. 4, 113 (2003)

TABLE 1-continued

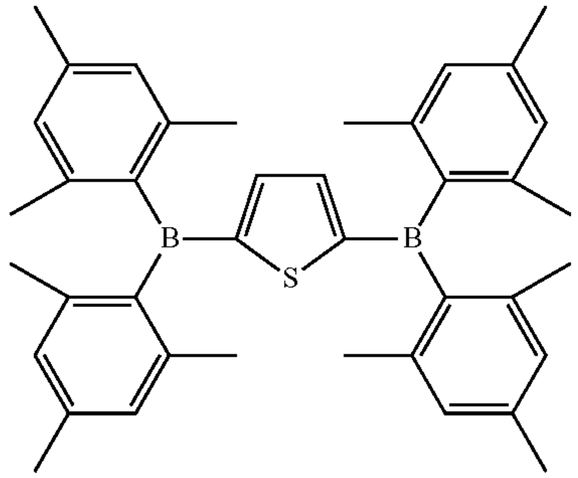
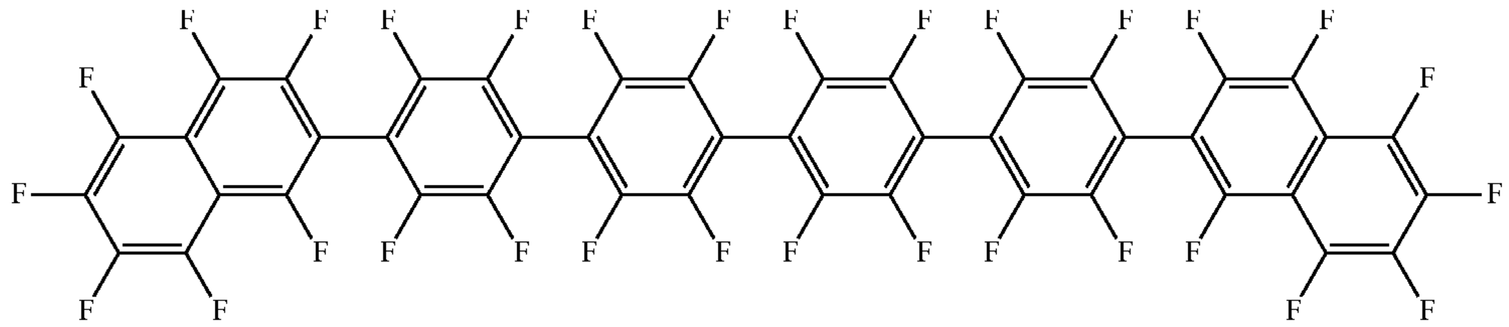
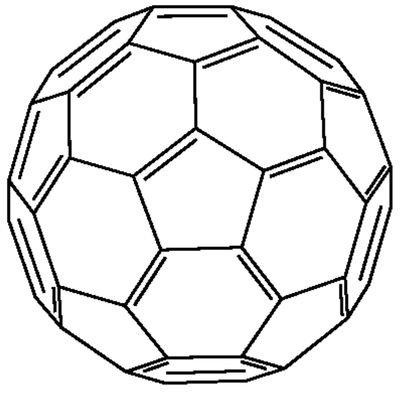
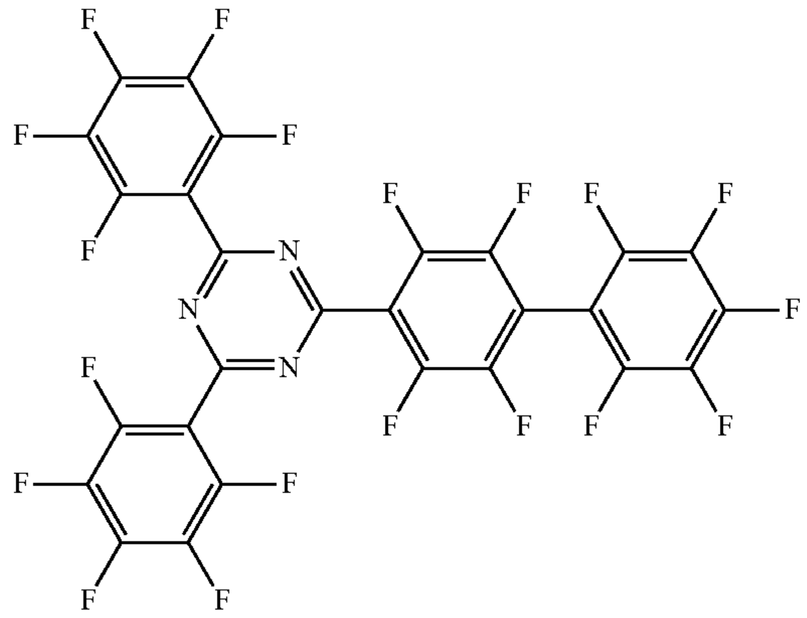
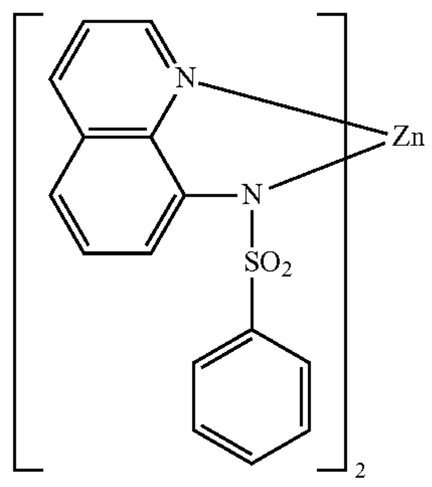
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
Fluorinated aromatic compounds		J. Am. Chem. Soc. 122, 1832 (2000)
Fullerene (e.g., C60)		US20090101870

TABLE 1-continued

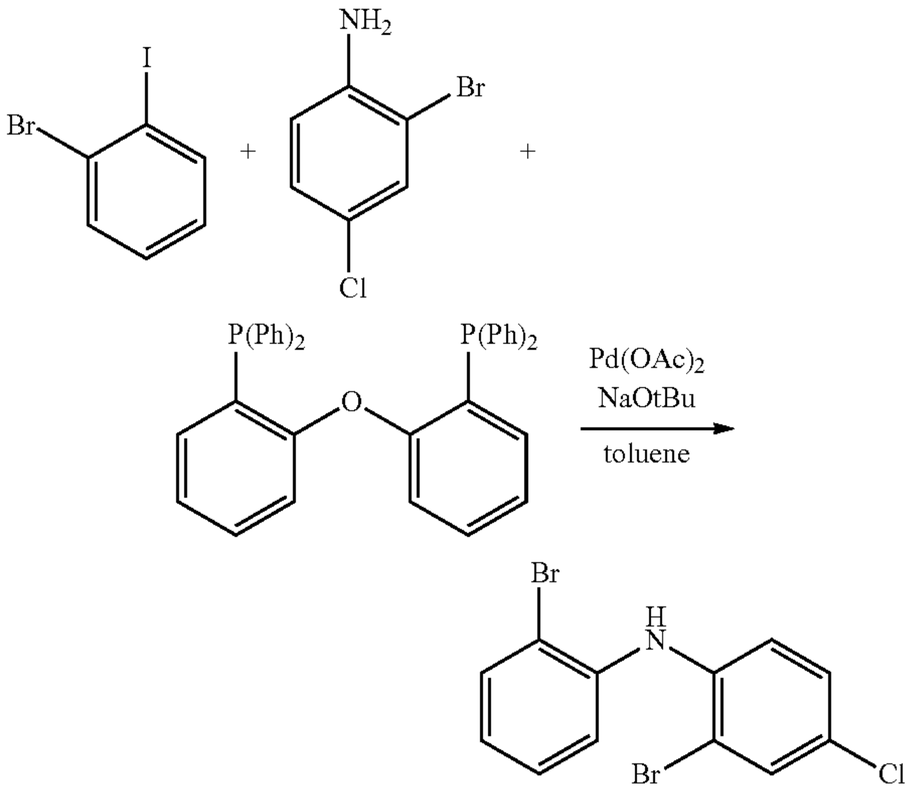
MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Triazine complexes		US20040036077
Zn (N^N) complexes		US6528187

EXPERIMENTAL

Synthesis of Heteroleptic Metal Complex

Preparation of
2-bromo-N-(2-bromophenyl)-4-chloroaniline

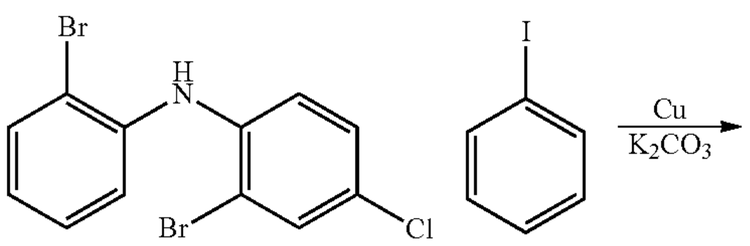
Sodium tert-butoxide (8.6 g, 89 mmol) was added to 1-bromo-2-iodobenzene (18 g, 64 mmol), 2-bromo-4-chloroaniline (13.1 g, 64 mmol), palladium(II) acetate (0.29 g, 1.3 mmol) and (oxybis(2,1-phenylene))bis(diphenylphosphine) (1.0 g, 1.9 mmol). The reaction flask was purged with nitrogen and 200 mL of toluene was added. The reaction was refluxed for 8 h in the absence of light.



After cooling to room temperature, the mixture was filtered through a pad of Celite®, washed with DCM and evaporated. The crude product was chromatographed on silica gel with 95:5 hexane:ethyl acetate to yield 19 g of 2-bromo-N-(2-bromophenyl)-4-chloroaniline. The product was confirmed by GC/MS and NMR.

Preparation of
2-bromo-N-(2-bromophenyl)-4-chloro-N-phenylaniline

Copper (1.67 g, 26.3 mmol) added to 2-bromo-N-(2-bromophenyl)-4-chloroaniline (19.0 g, 52.6 mmol), iodobenzene (5.86 mL, 52.6 mmol) and potassium carbonate (7.26 g, 52.6 mmol). The reaction flask was purged with nitrogen and heated up to 200° C. (outside temperature) for 24 h.



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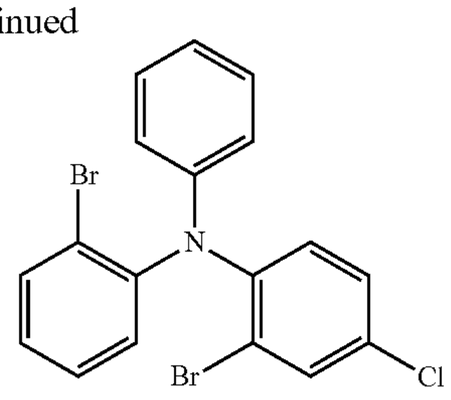
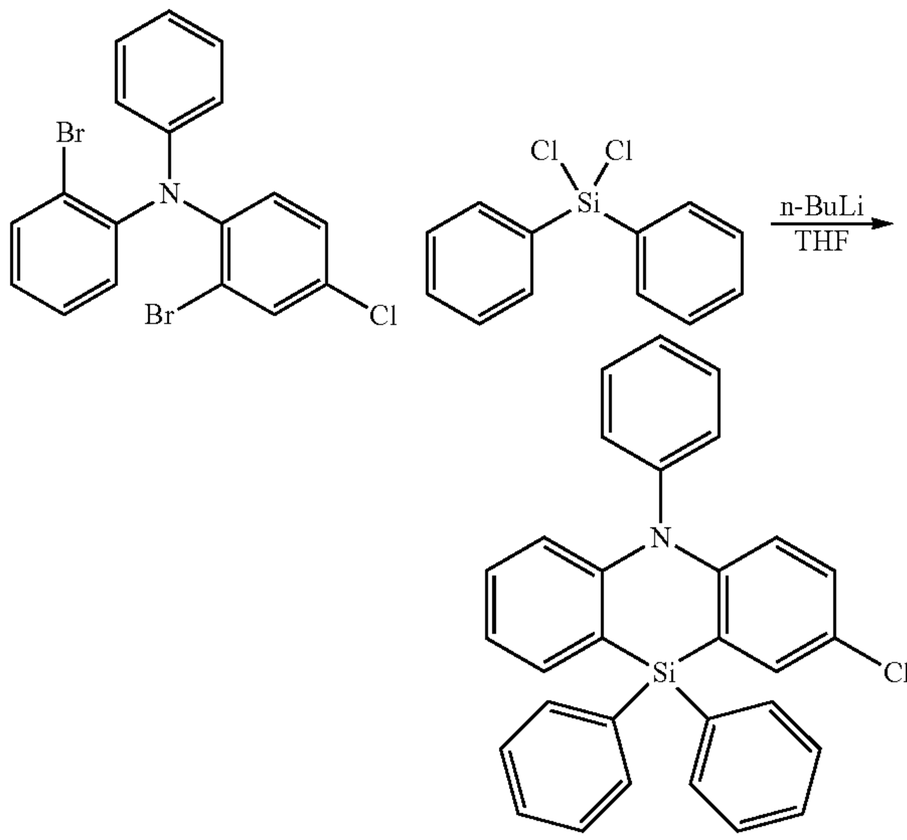


Another two equivalents of iodobenzene were added and the reaction mixture was heated to 200° C. for an additional 24 h. After cooling to room temperature, 50 mL of ethyl acetate was added. The mixture was stirred for 10 min, then filtered and washed with ethyl acetate. The solvent was evaporated and excess iodobenzene was removed by Kugelrohr distillation. The crude product was chromatographed on silica gel with 5-10% DCM in hexane to give 12 g of 2-bromo-N-(2-bromophenyl)-4-chloro-N-phenylaniline. The product was confirmed by NMR.

Preparation of 2-chloro-5,10,10-triphenyl-5,1-dihydrodibenzo[b,e][1,4]azasiline

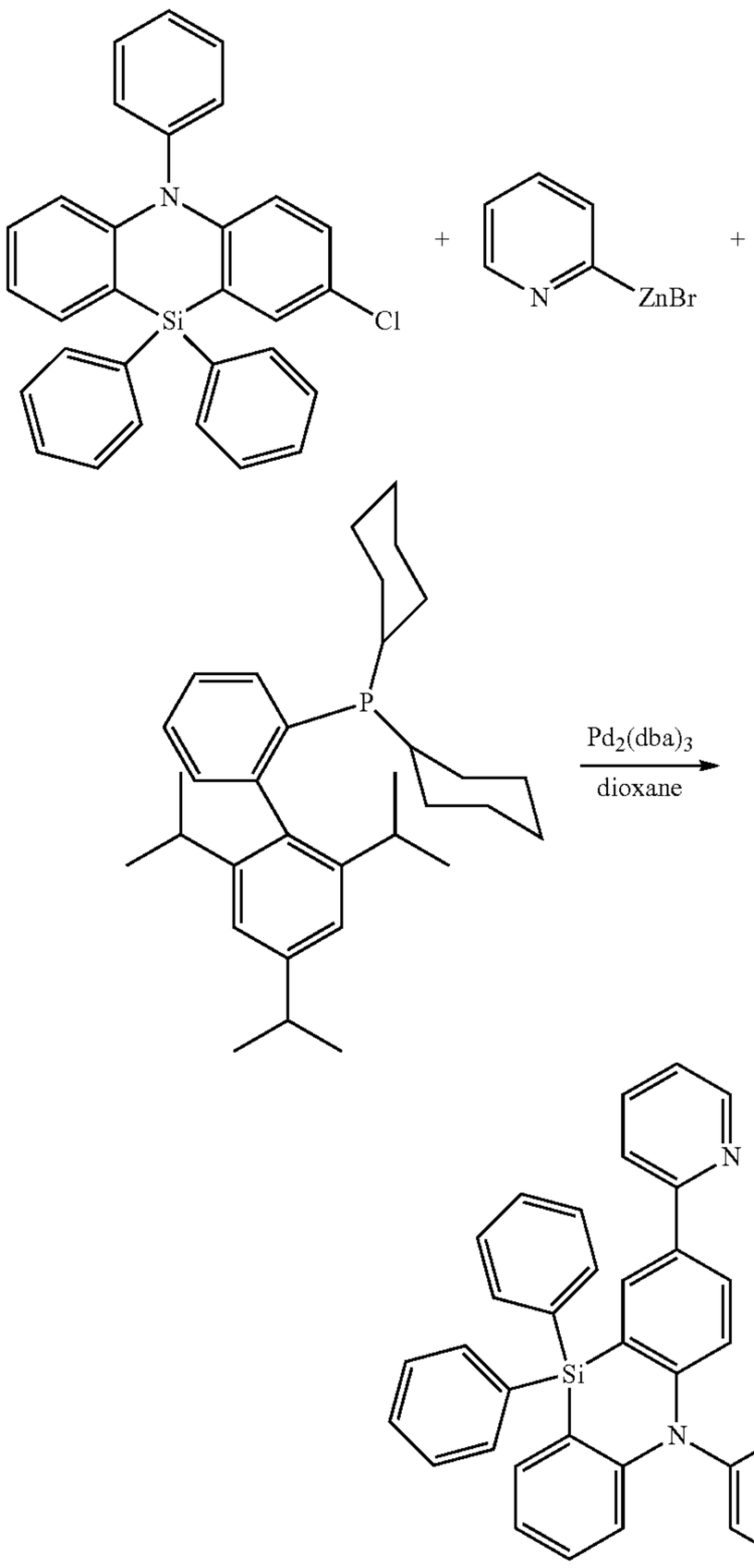
n-Butyl lithium (17.4 mL, 43.4 mmol) was added slowly to 2-bromo-N-(2-bromophenyl)-4-chloro-N-phenylaniline (9.5 g, 21.71 mmol) in 200 mL of THF at −78° C. The reaction was stirred at −78° C. for two hours. Dichlorodiphenylsilane (4.9 mL, 23.9 mmol) was dissolved in 50 mL of THF and added dropwise to the reaction very slowly. The reaction was then allowed to warm up to room temperature overnight.



200 mL of water was added to the reaction mixture, which was then stirred for 20 minutes before being extracted 3×100 mL with ethyl acetate. The combined organic layers were washed with brine and dried over sodium sulfate. After removal of the solvent, the crude product was chromatographed on a silica gel column pretreated with 80:20 hexane:triethylamine. The product was obtained by elution with 5-20% DCM in hexane to give 6.5 g of 2-chloro-5,10,10-triphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline. The product was confirmed by NMR.

Preparation of 5,10,10-triphenyl-2-(pyridin-2-yl)-5,10-dihydrodibenzo[b,e][1,4]aza-siline

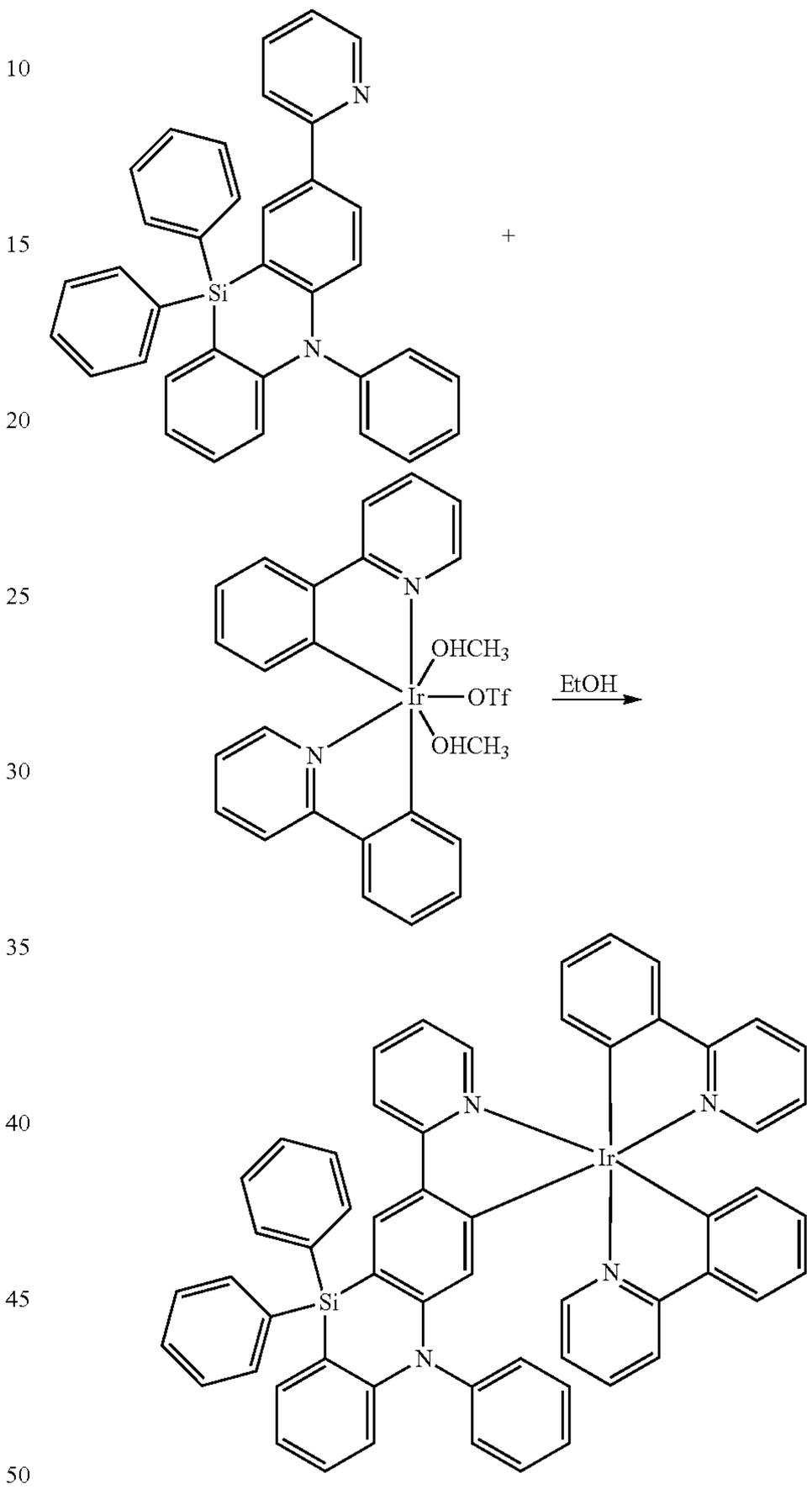
$Pd_2(dba)_3$ (0.42 g, 0.46 mmol) and dicyclohexyl(2',4',6'-triisopropyl-[1,1'-biphenyl]-2-yl)phosphine (0.88 g, 1.8 mmol) in 50 mL degased dioxane was heated to reflux for 20 min. 2-Chloro-5,10,10-triphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (5.3 g, 11.5 mmol) in 50 mL degased dioxane was syringed into the reaction and allowed to reflux for 15 min. Pyridin-2-ylzinc(II) bromide (46.0 mL, 23.0 mmol, 0.5 M in THF) was added dropwise to the reaction and subsequently the reaction mixture was heated to reflux for 2 h.



The reaction was cooled to room temperature, and 100 mL of saturated Na_2CO_3 solution was added to the reaction, and the contents extracted 3×100 mL with ethyl acetate. The combined organics were dried over sodium sulfate and evaporated. The crude product was chromatographed on silica gel with 10-40% ethyl acetate in hexane. The product was then recrystallized from DCM/hexane followed by a second recrystallization from DCM/ethanol to yield 4.3 g of 5,10,10-triphenyl-2-(pyridin-2-yl)-5,10-dihydrodibenzo[b,e][1,4]aza-siline. The product was confirmed by NMR.

Preparation of Heteroleptic Metal Complex

5,10,10-triphenyl-2-(pyridin-2-yl)-5,10-dihydrodibenzo[b,e][1,4]azasiline (4.2 g, 8.4 mmol) and the iridium triflate complex (2 g, 2.8 mmol) were heated to relux in 25 mL EtOH for 16 hours.



After cooling the reaction to room temperature, it was filtered through a Celite® plug and washed with ethanol and hexane. The product on the plug was washed off with DCM and the filtrate evaporated. The crude product was chromatographed on silica gel with 30-100% DCM in hexane to yield 1.3 g of product. The still impure material was chromatographed on a silica gel column pretreated with 80:20 hexane:triethylamine. The product was obtained by elution with 20-40% EtOAc in hexane. The material was further lixiviated with isopropanol to give 0.5 g of the desired metal complex. The product was confirmed by NMR and LC/MS. The complex showed phosphorescent emission with λ_{max} of 524 nm and transient lifetime of 8.06 μs at room temperature in 2-MeTHF solution.

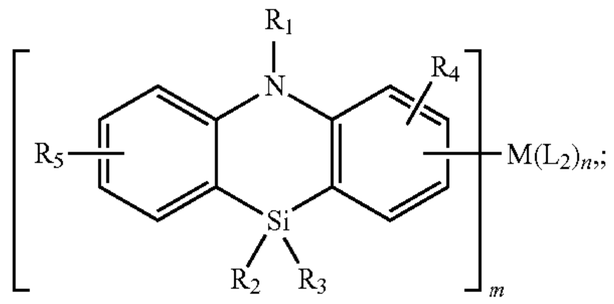
It is understood that the various embodiments described herein are by way of example only, and are not intended to

limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

We claim:

1. A compound having a structure of Formula II:

Formula II



wherein metal M has an atomic weight higher than 40;

wherein R_5 represents mono, di, tri, tetra substitutions or no substitution;

wherein R_4 represents mono, di, or tri substitutions;

wherein each L_2 is a ligand coordinated to the metal M;

wherein each L_2 can be the same or different;

wherein R_1, R_2, R_3, R_4, and R_5 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;

wherein one R_4 is coordinated to the metal M;

wherein any two adjacent R_2, R_3, R_4, and R_5 are optionally joined to form a ring, which may be further substituted;

wherein the metal M does not form a direct bond with the N or the Si of Formula II;

wherein any of R_1, R_2, R_3, and R_4 are optionally linked to L_2 to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand;

wherein m is a value from 1 to the maximum number of ligands that may be attached to the metal M; and

wherein m+n is the maximum number of ligands that may be attached to the metal M.

2. The compound of claim **1**, wherein the metal M is a metal selected from the group consisting of Ir, Pt, Re, Os, Ru, Rh, Pd, Cu, Ag, and Au.

3. The compound of claim **1**, wherein the metal M is Ir.

4. The compound of claim **1**, wherein the metal M is Pt.

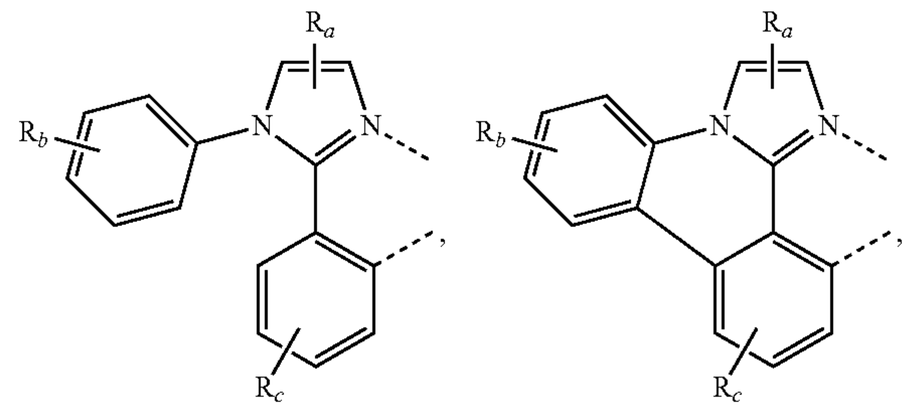
5. The compound of claim **1**, wherein at least one of R_1, R_2, and R_3 is aryl or substituted aryl.

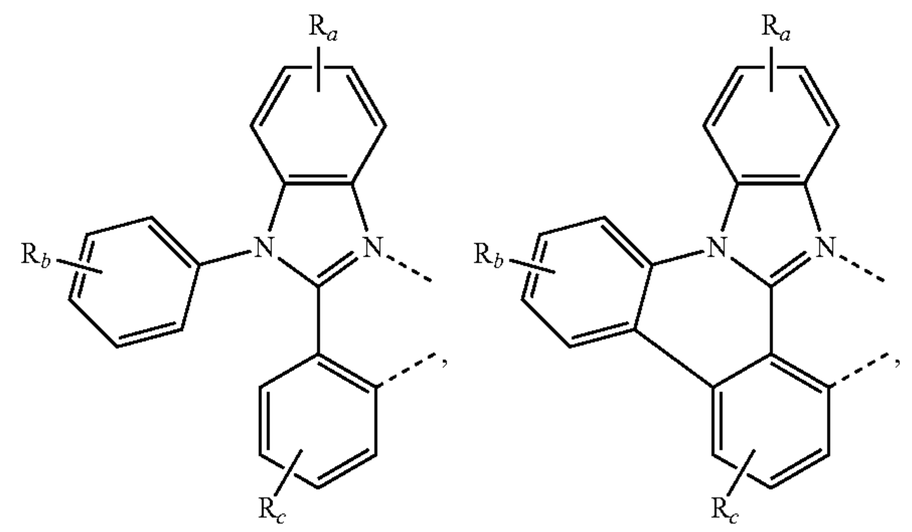
6. The compound of claim **5**, wherein at least one of R_1, R_2, and R_3 is phenyl or substituted phenyl.

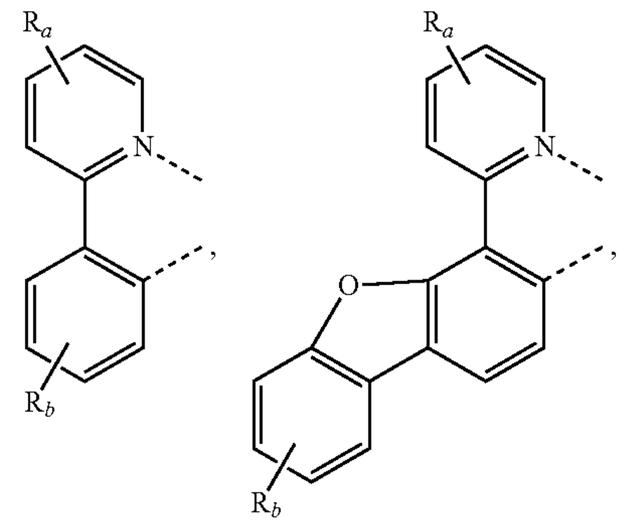
7. The compound of claim **1**, wherein the compound is homoleptic.

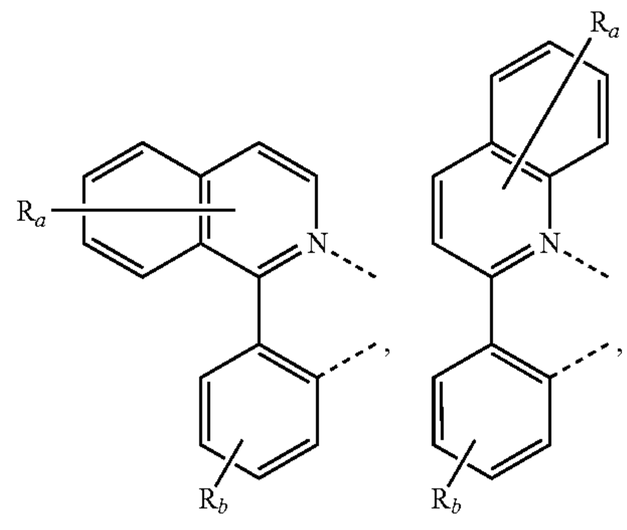
8. The compound of claim **1**, wherein the compound is heteroleptic.

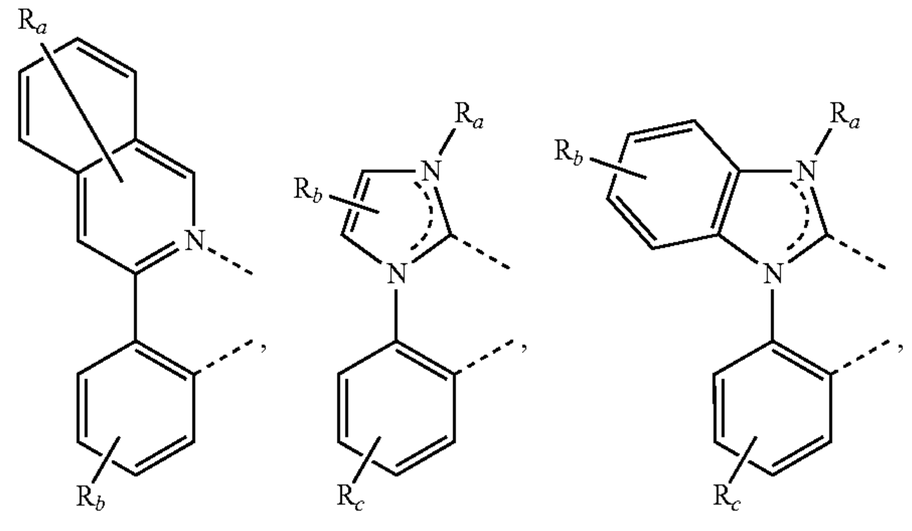
9. The compound of claim **8**, wherein L_2 or part of L_2 if L_2 is more than bidentate is selected from the group consisting of:











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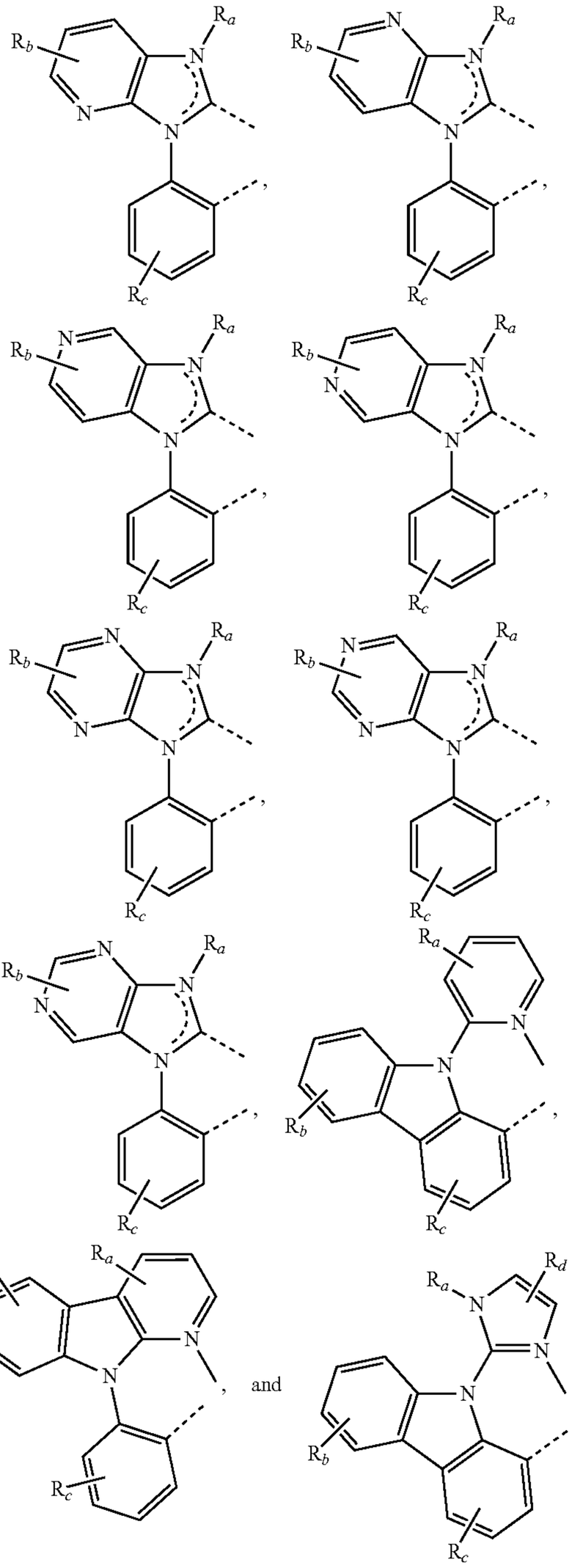


wherein R_a, R_b, R_c, and R_d may represent mono, di, tri, or tetra substitution, or no substitution;

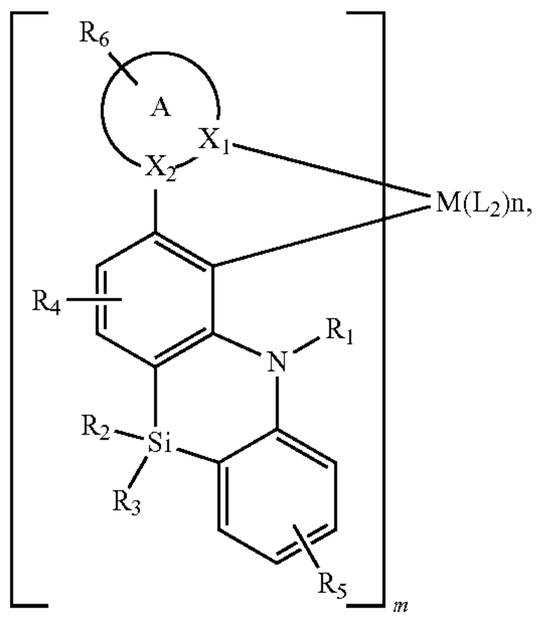
wherein R_a, R_b, R_c, and R_d are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfanyl, sulfonyl, phosphino, and combinations thereof; and

wherein two adjacent substituents of R_a, R_b, R_c, and R_d are optionally joined to form a fused ring or form a multidentate ligand.

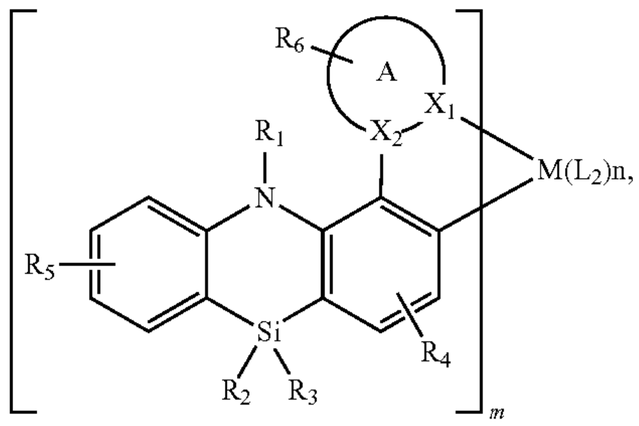
10. The compound of claim **1**, wherein at least one of R_1, R_2, and R_3 are linked to L_2 to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand.

11. The compound of claim **1**, wherein the compound is selected from the group consisting of:

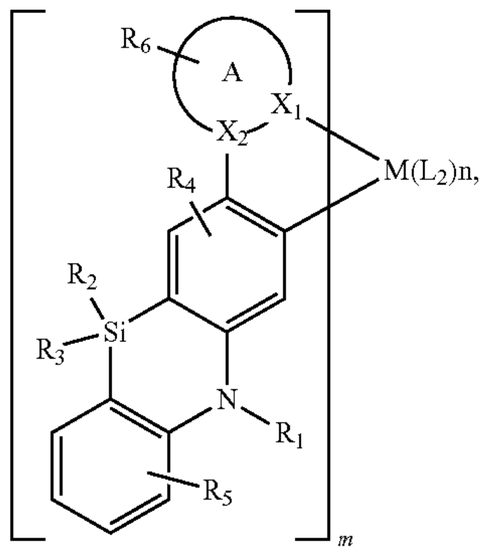
GS 2



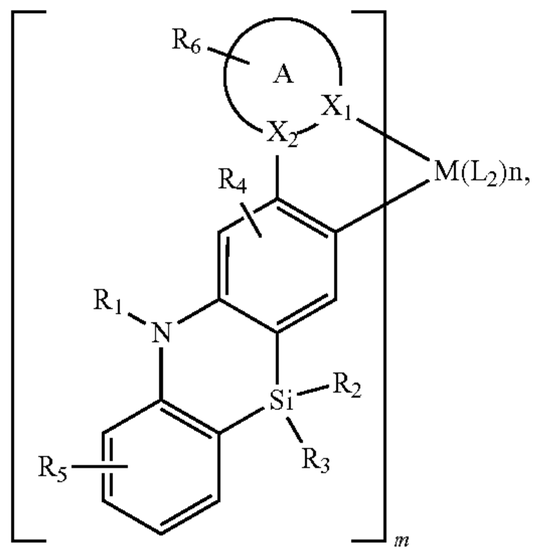
GS 3



GS 4



GS 5



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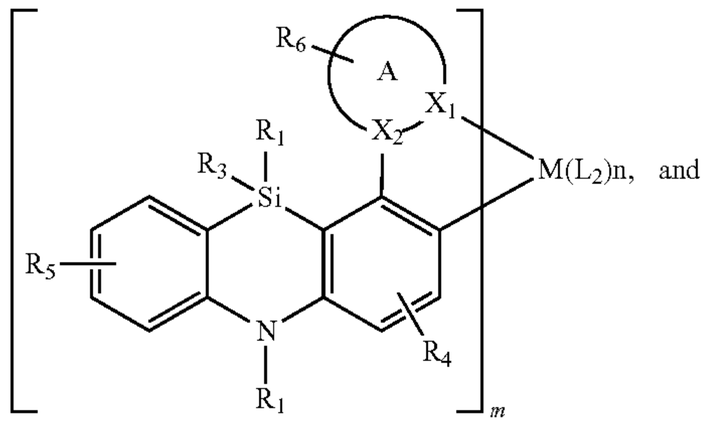
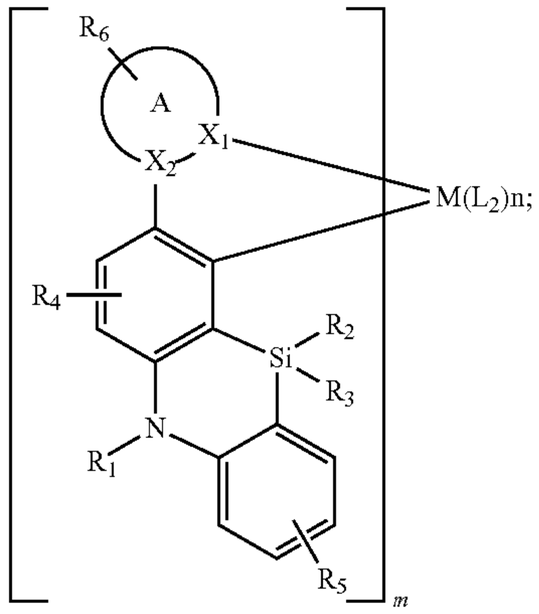


and



wherein X_1, X_2 is selected from the group consisting of C, N, O, P, S, and B;

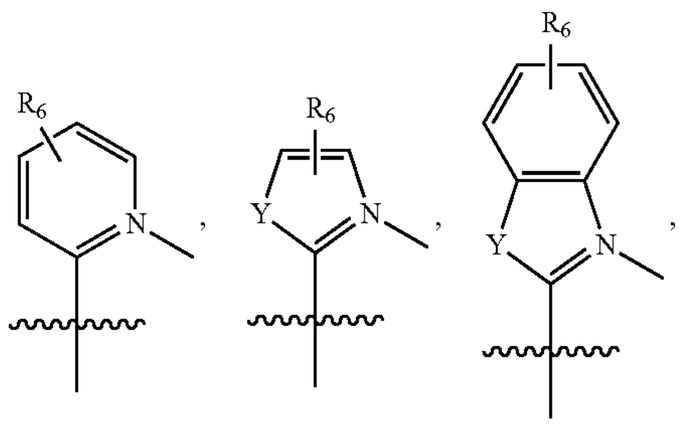
wherein A is a 5-membered or 6-membered carbocyclic or heterocyclic ring;

wherein R_6 represents mono, di, tri, tetra substitutions or no substitution;

wherein R_6 is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein any two adjacent R_1, R_2, R_3, R_4, R_5, and R_6 are optionally joined to form a ring, which may be further substituted.

12. The compound of claim **11**, wherein A is selected from the group consisting of:



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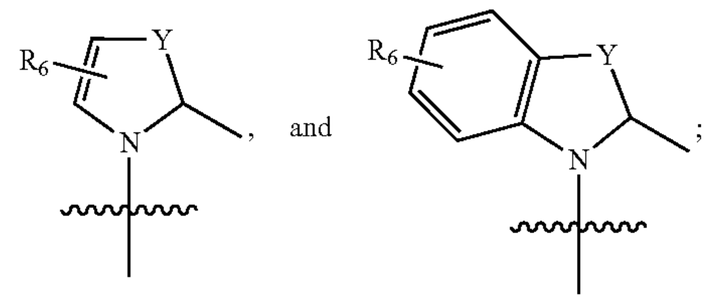
GS 6



and

;

wherein Y is selected from the group consisting of BR, NR, PR, O, S, Se, C═O, S═O, SO_2, CRR', SiRR', and GeRR;

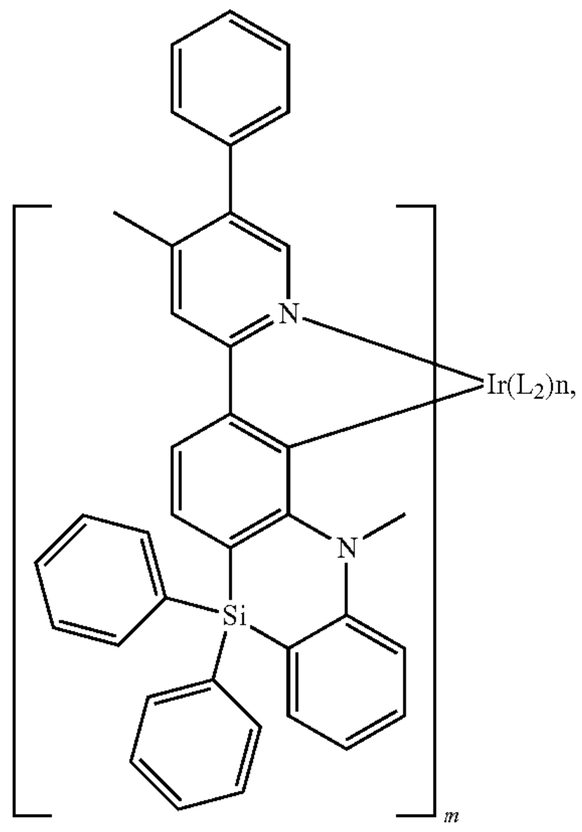
GS 7

wherein R, R' are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfanyl, sulfonyl, phosphino, and combinations thereof; and

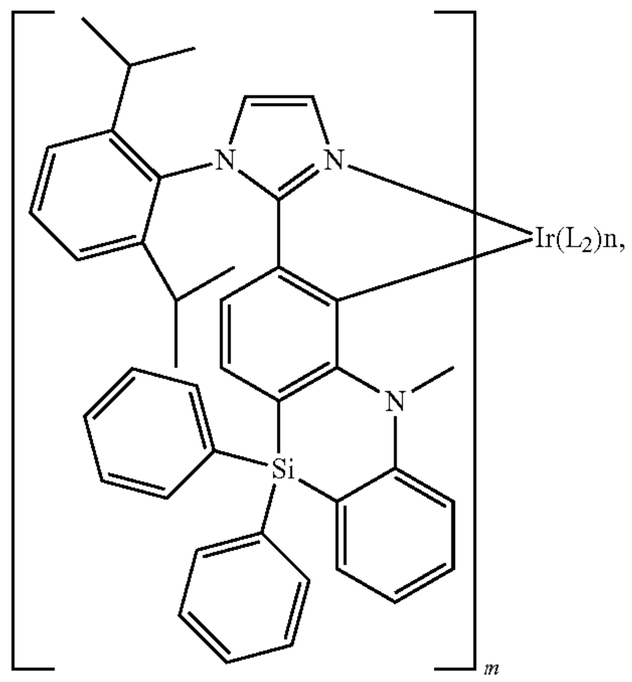
wherein R, R' are optionally joined to form a ring with any adjacent substituent.

13. The compound of claim **1**, wherein the compound is selected from the group consisting of:

Compound 2-1



Compound 2-2



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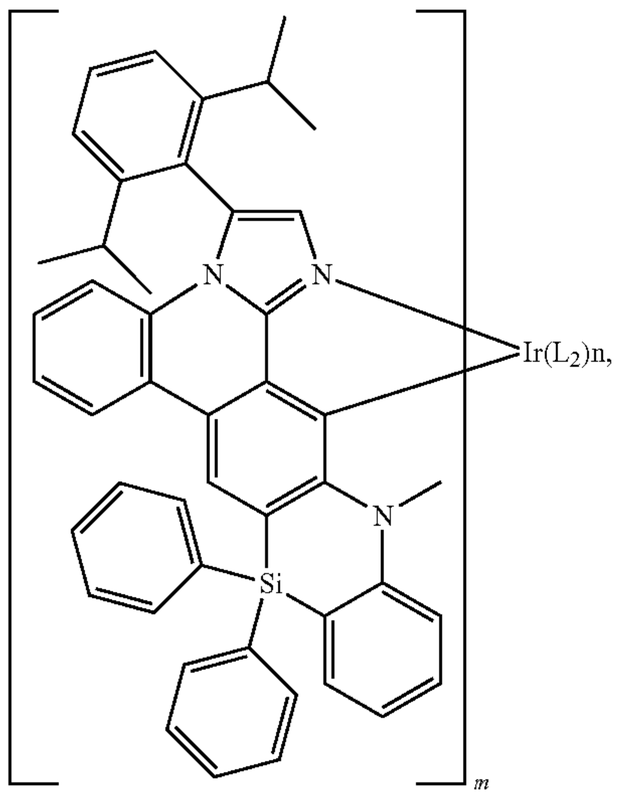
Compound 2-3



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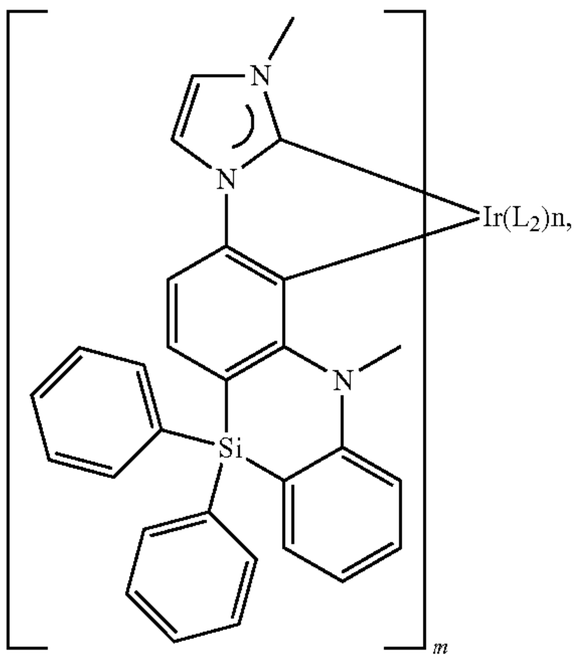
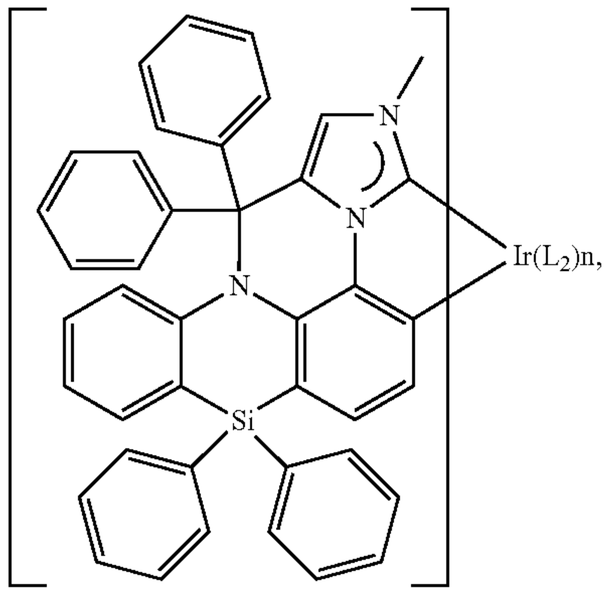
Compound 2-4



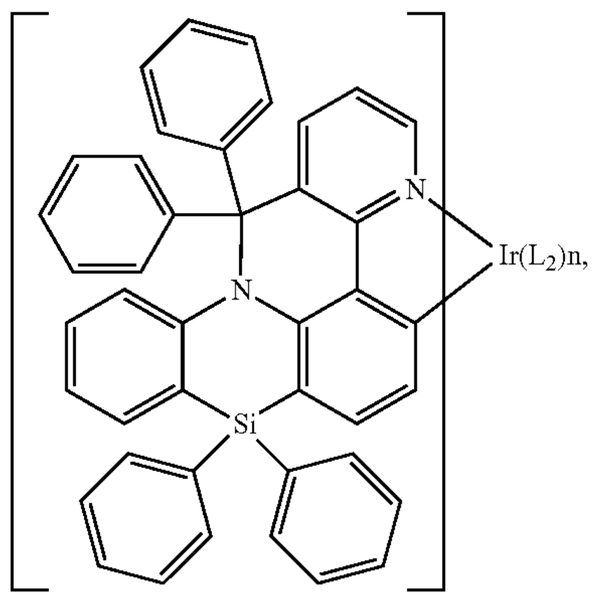
Compound 3-1

-continued

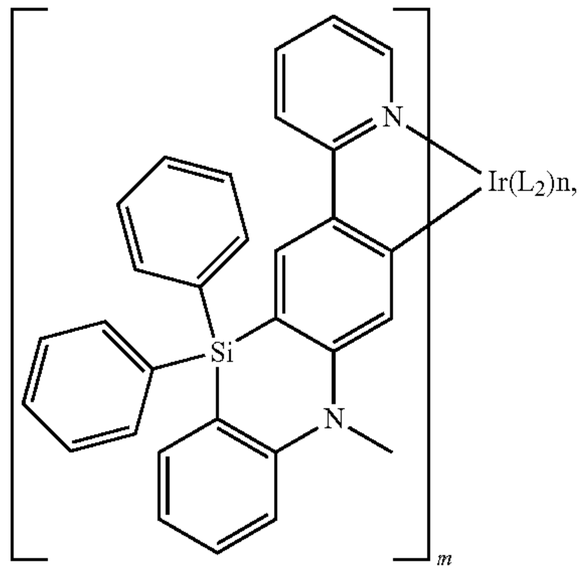
Compound 3-2



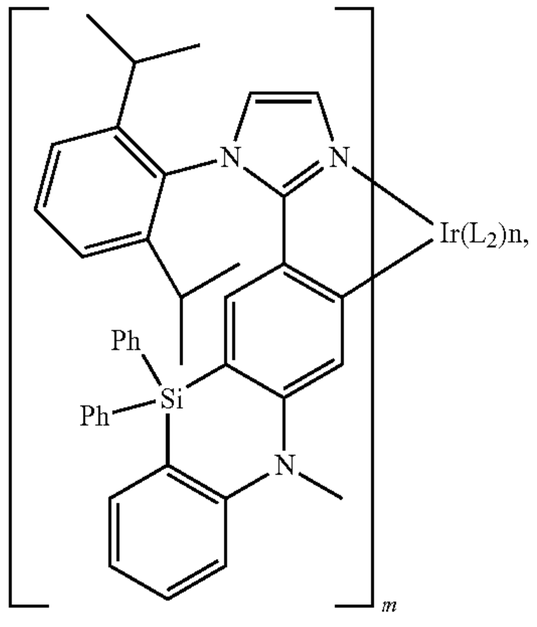
Compound 3-3



Compound 4-1



Compound 4-2



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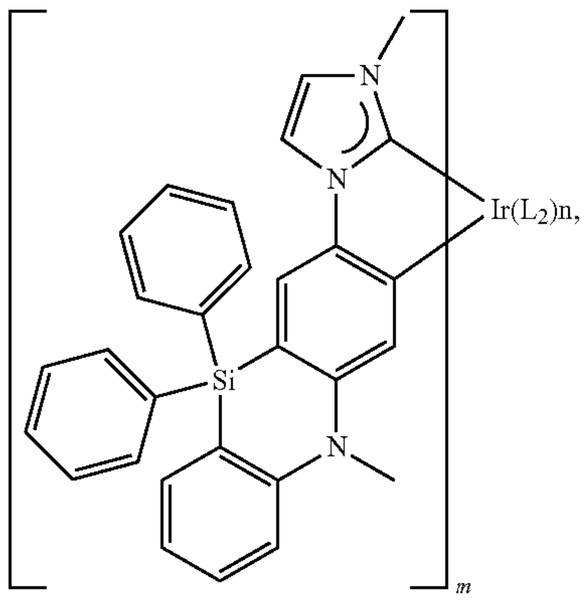
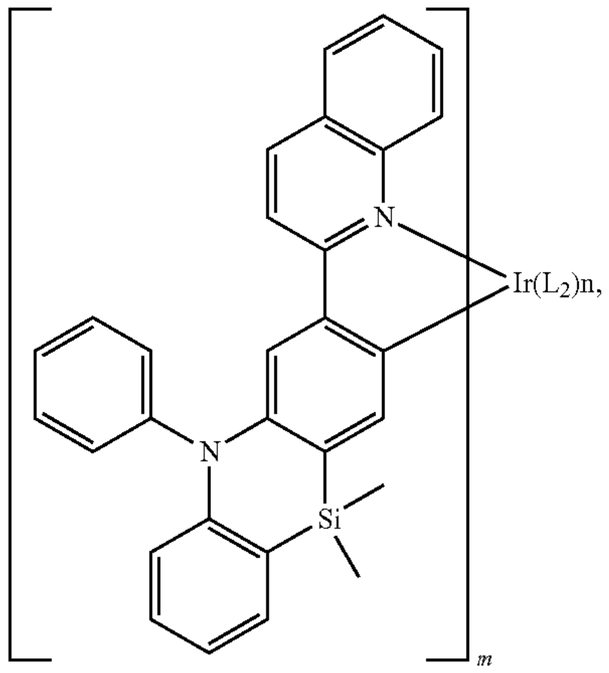
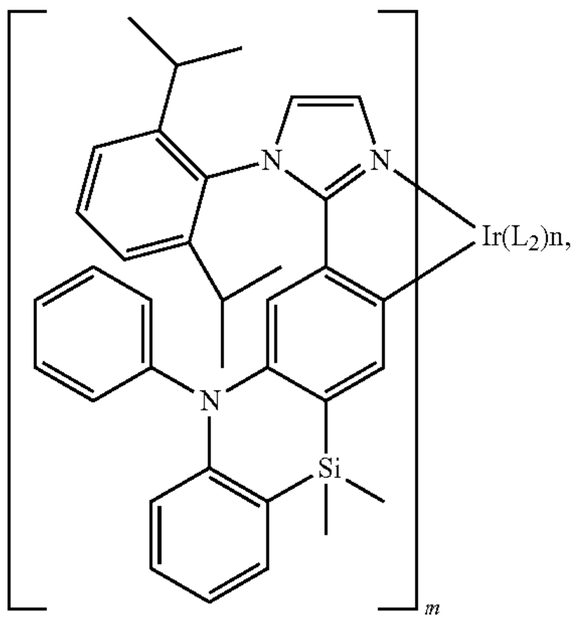
Compound 4-3



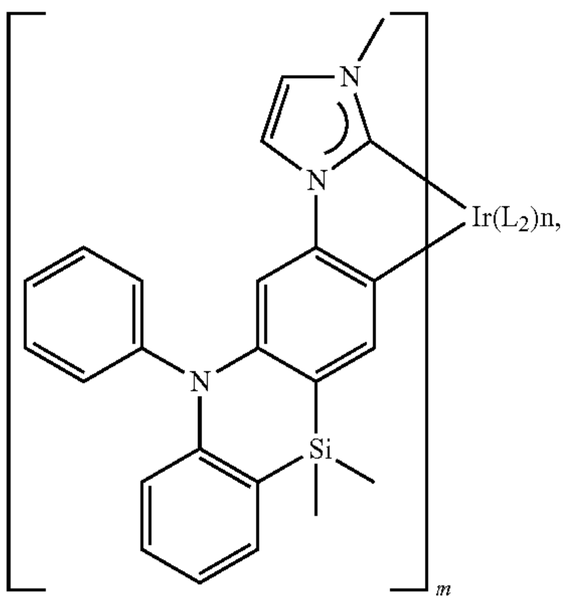
Compound 5-1



Compound 5-2



Compound 5-3



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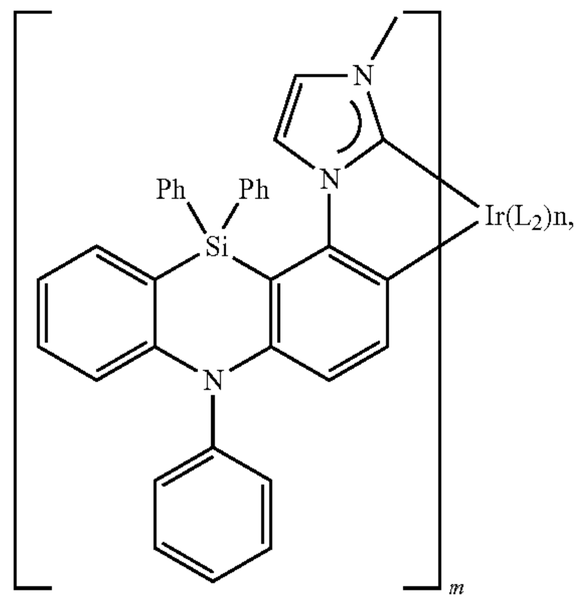
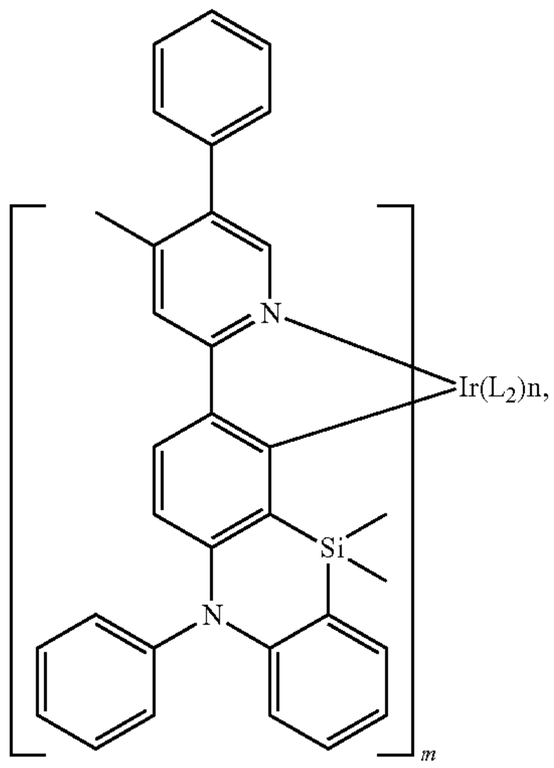
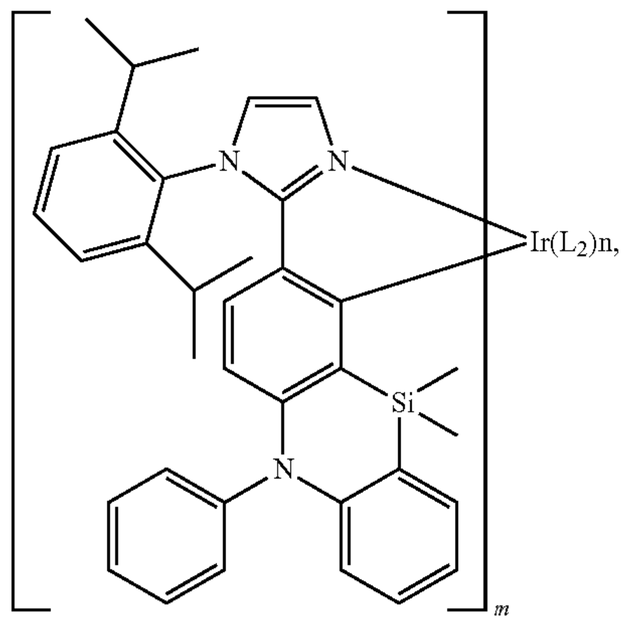
Compound 6-1



Compound 7-1



Compound 7-2



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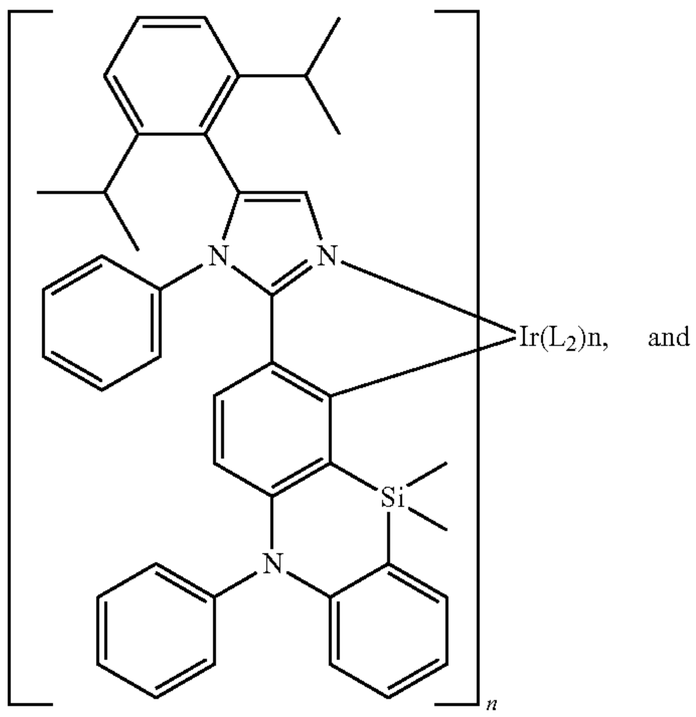
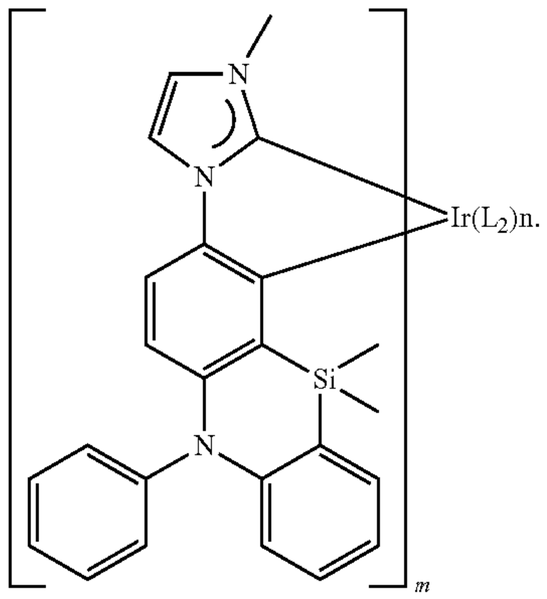
Compound 7-3



and

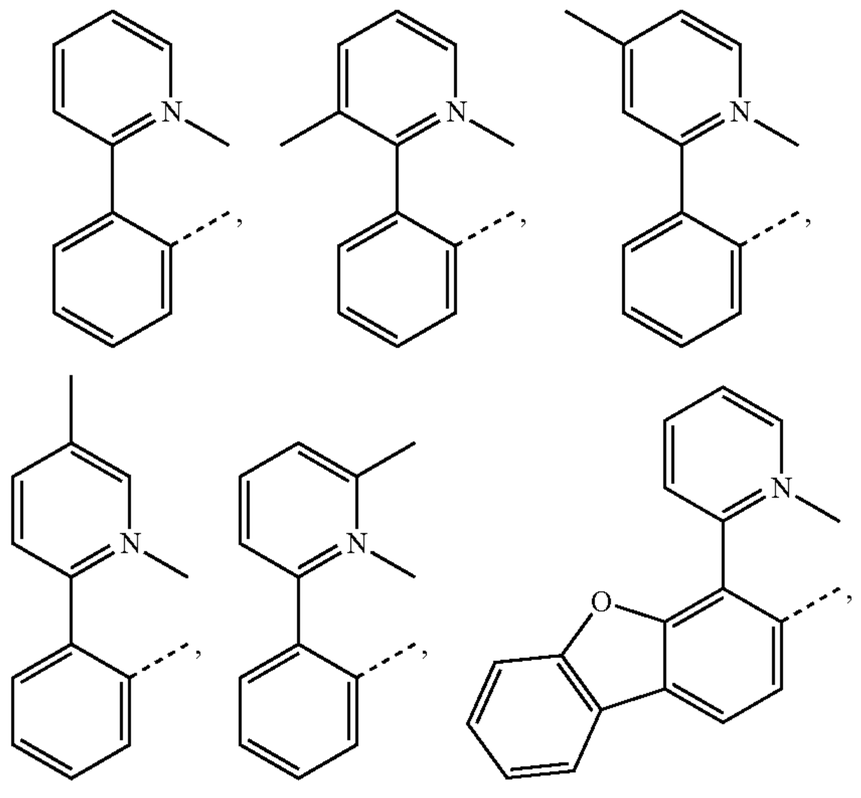
Compound 7-4



14. The compound of claim **13**, wherein m is 3, and n is 0.

15. The compound of claim **13**, wherein m is 1, and n is 2.

16. The compound of claim **13**, wherein L_2 is selected from the group consisting of:



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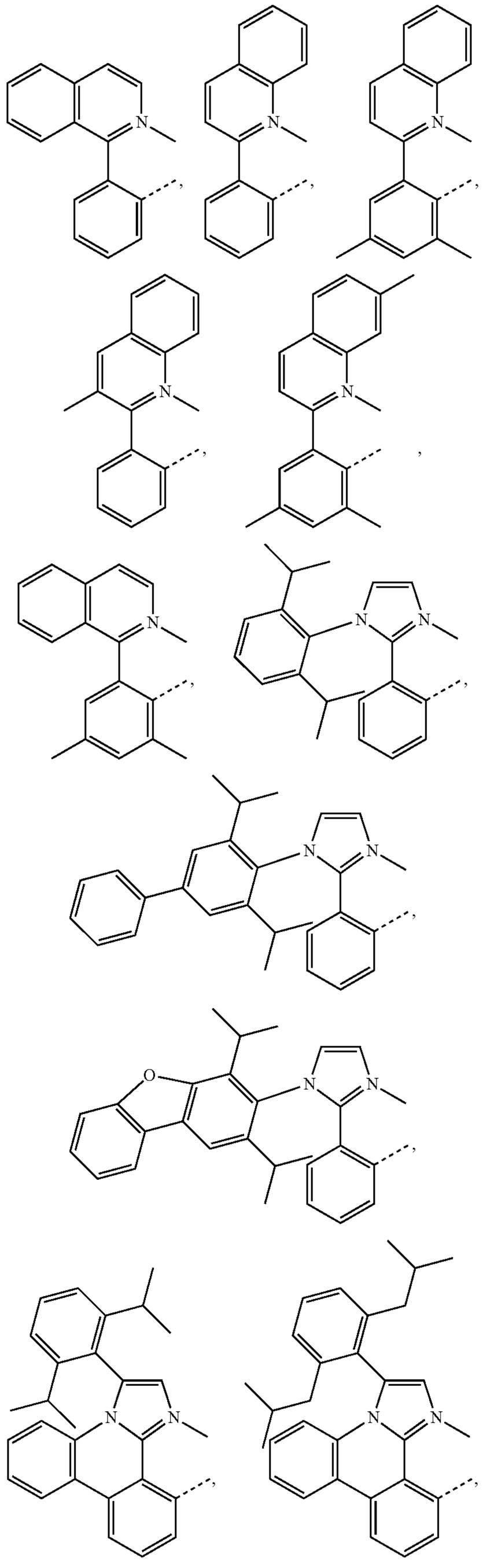

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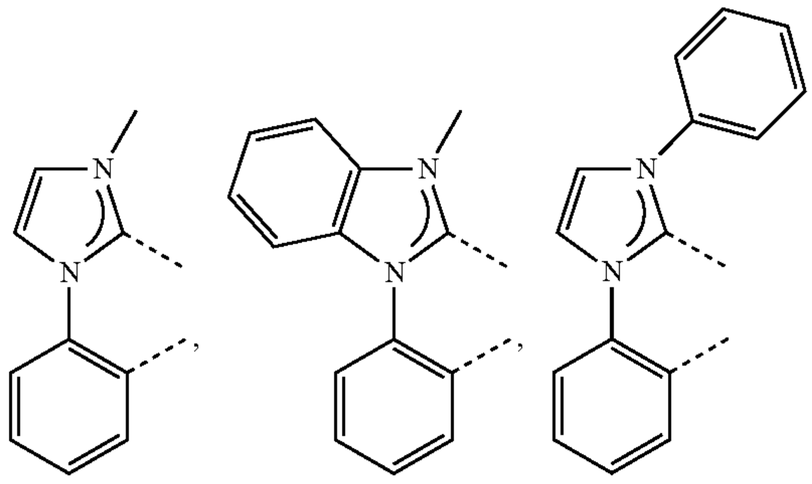
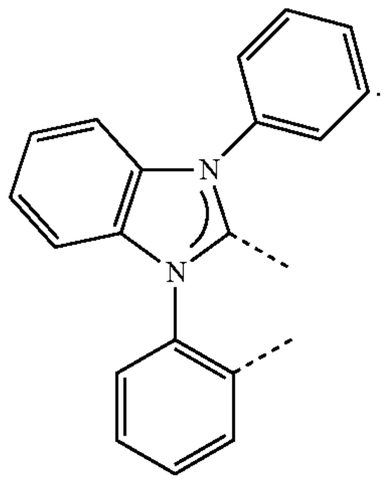
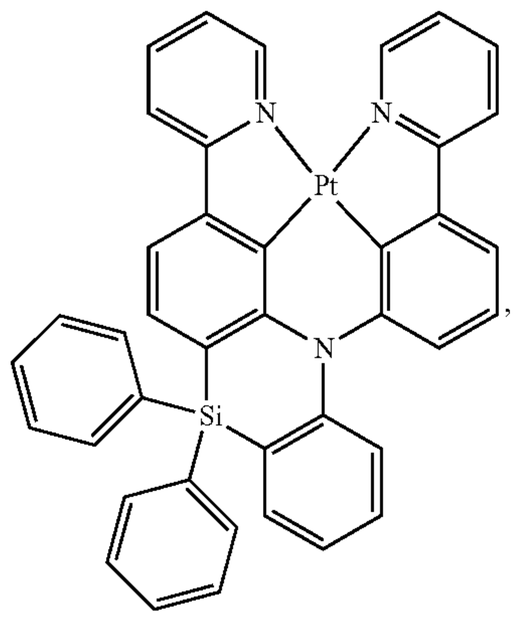


, and

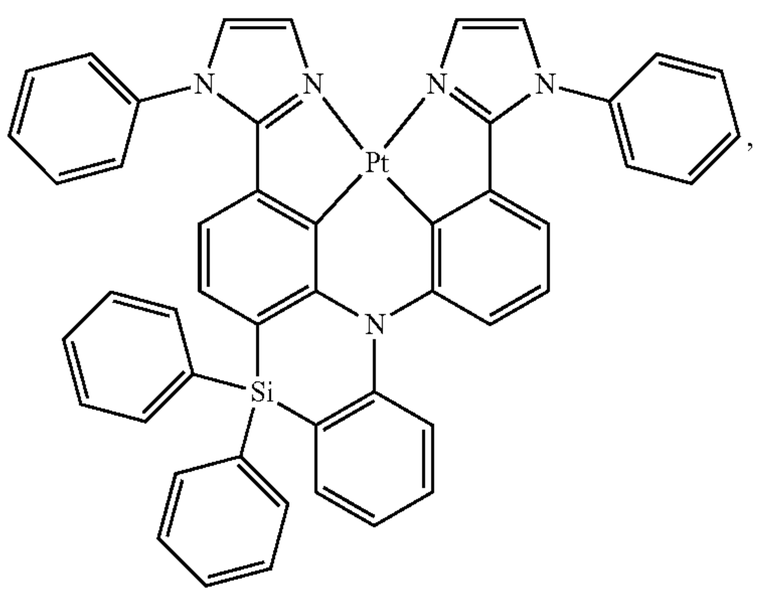


17. The compound of claim **1**, wherein the compound is selected from the group consisting of:

Compound 2-11



Compound 2-12



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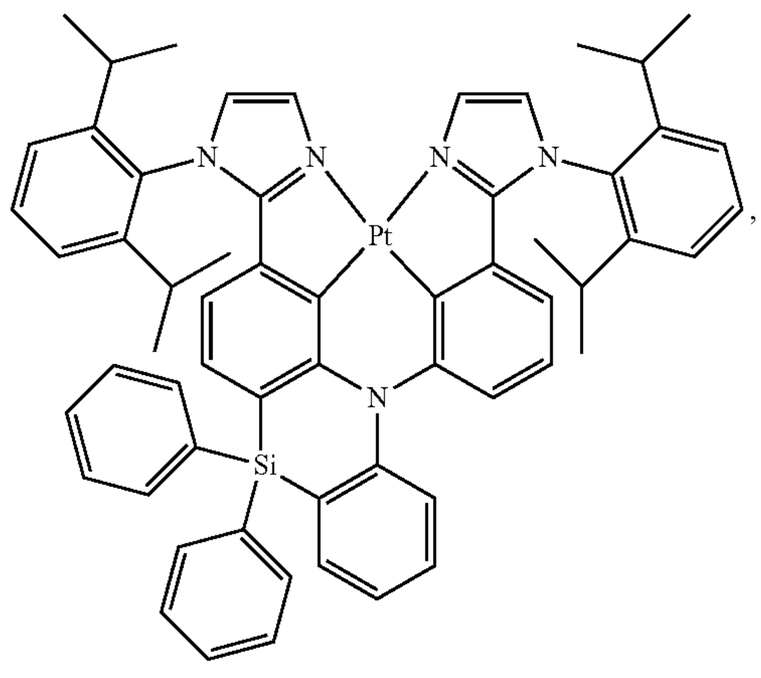
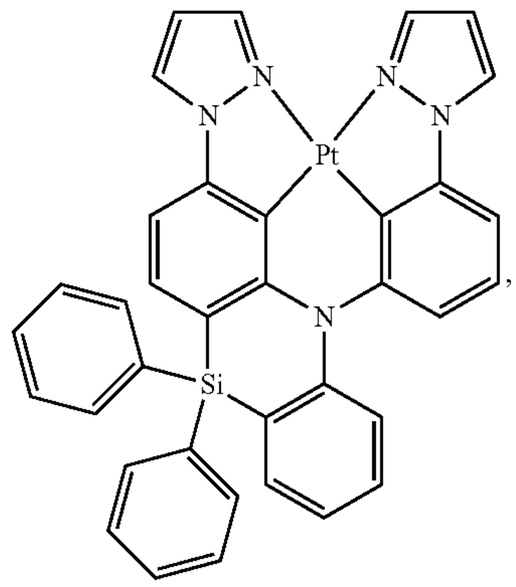
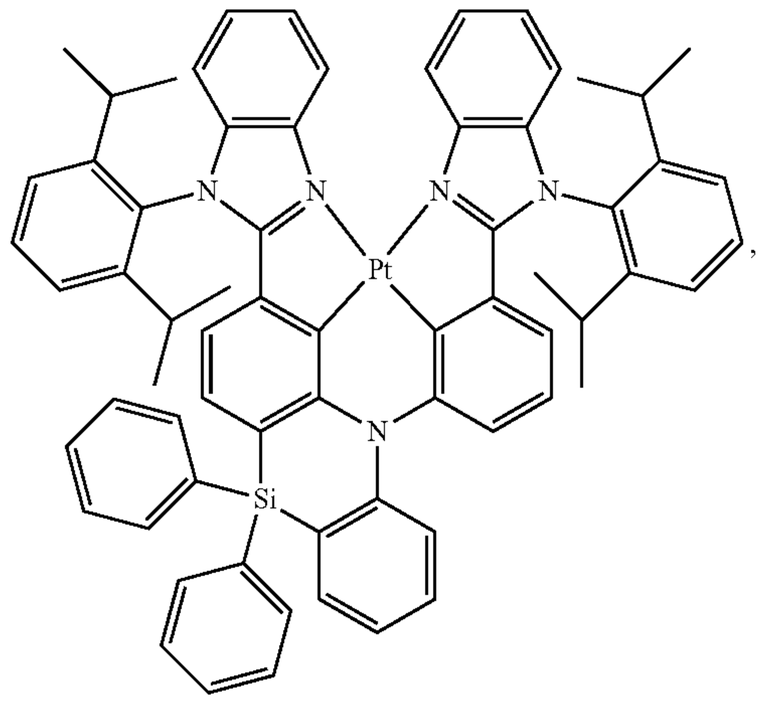
Compound 2-13



Compound 2-14



Compound 2-15



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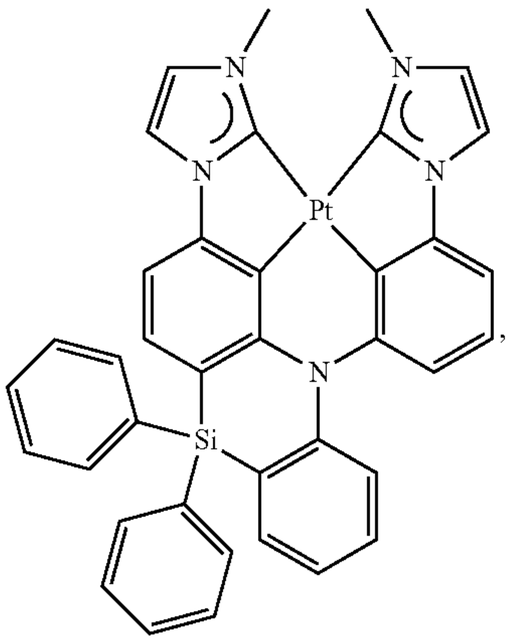
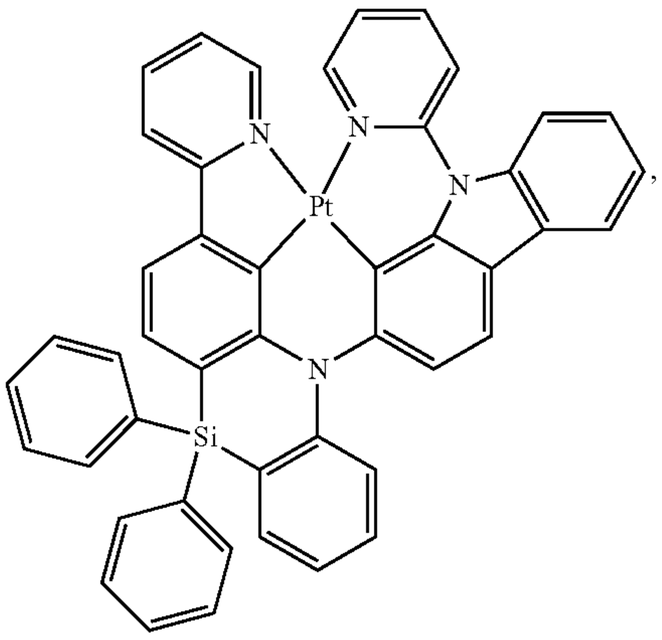
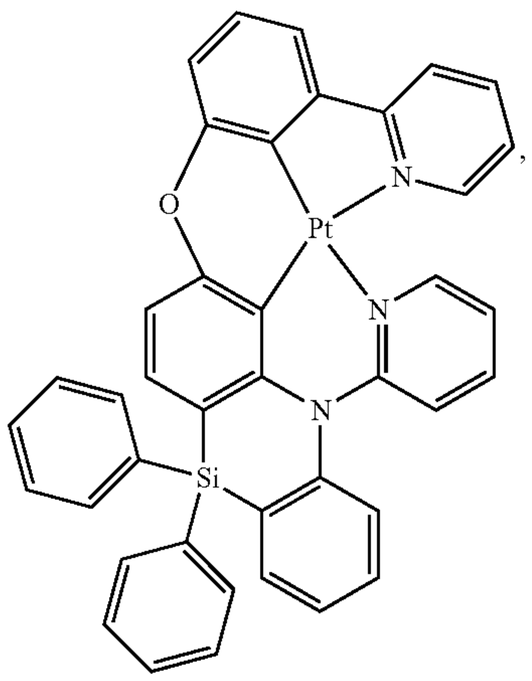
Compound 2-16



Compound 2-17



Compound 2-18



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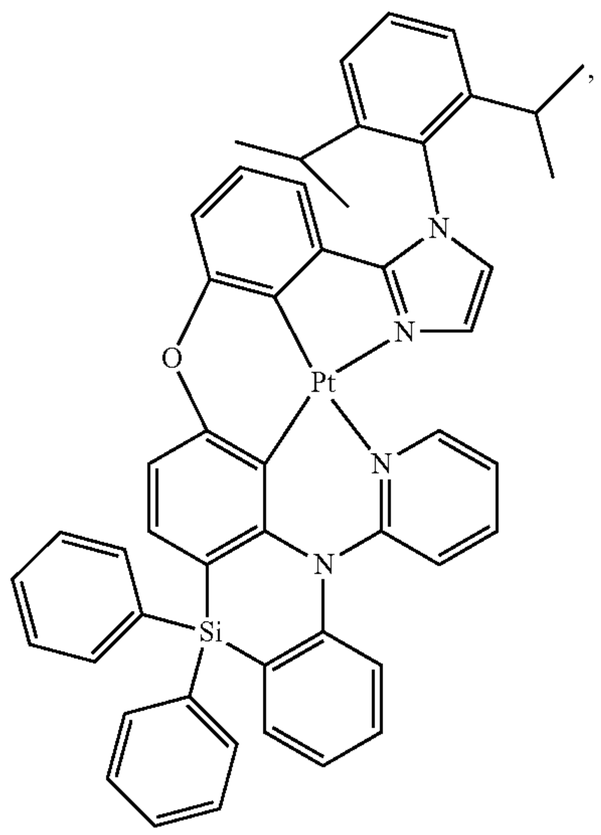
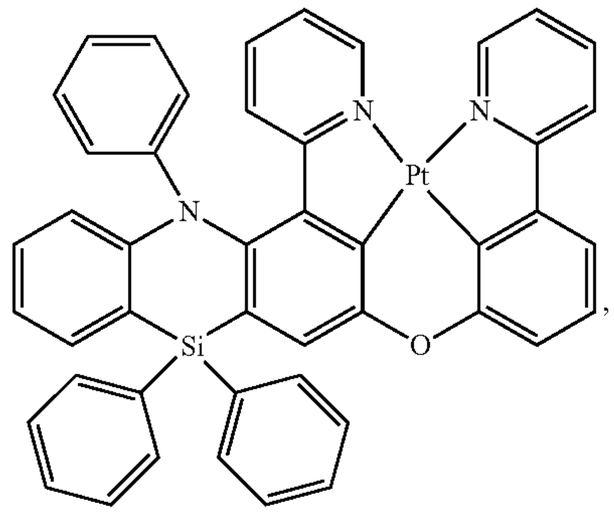
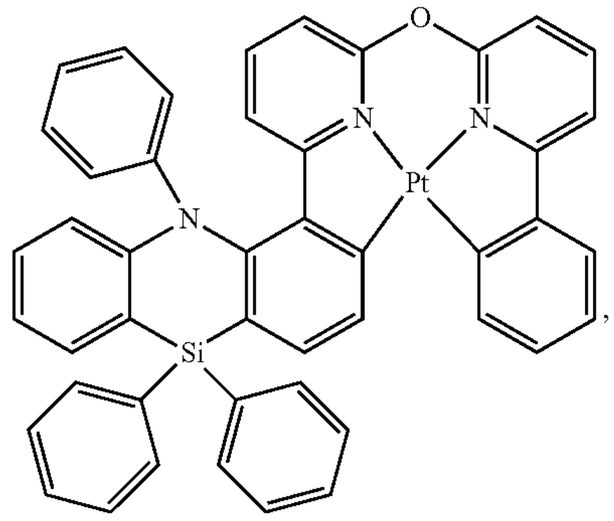
Compound 2-19



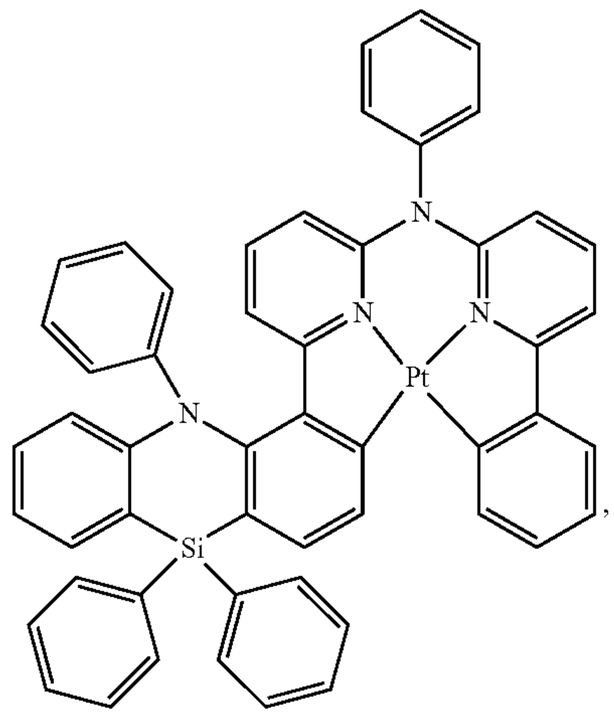
Compound 3-11



Compound 3-12



Compound 3-13



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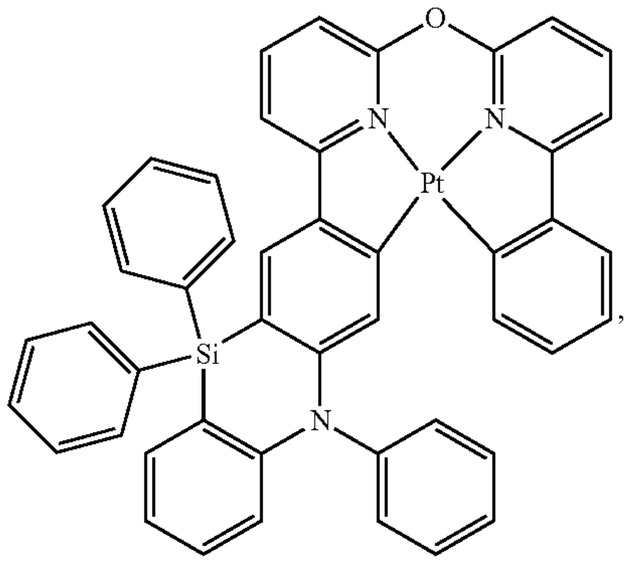
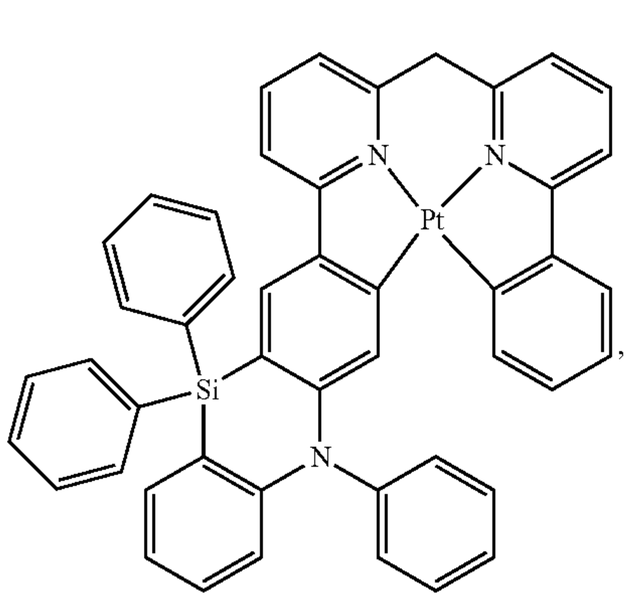
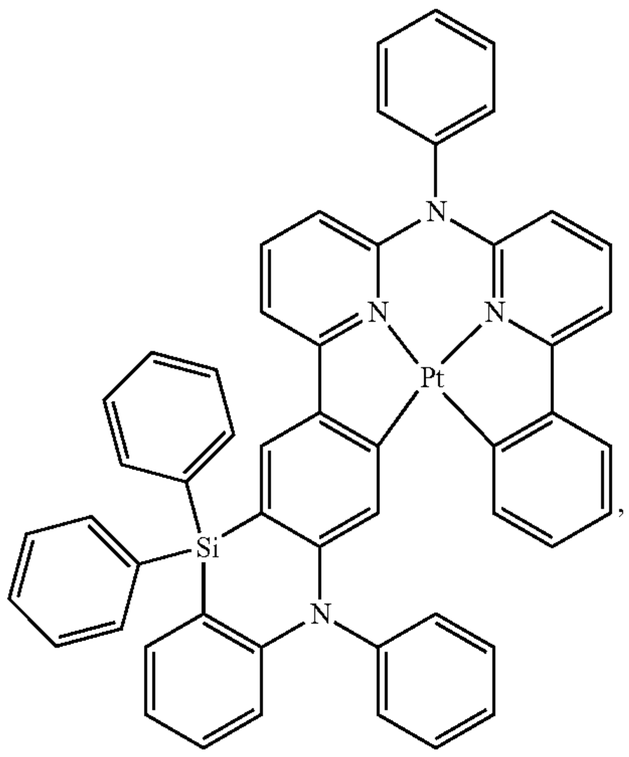
Compound 4-11



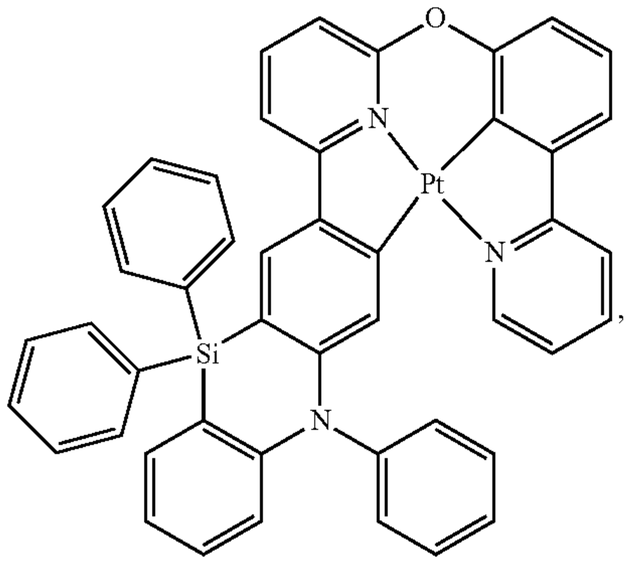
Compound 4-12



Compound 4-13



Compound 4-14



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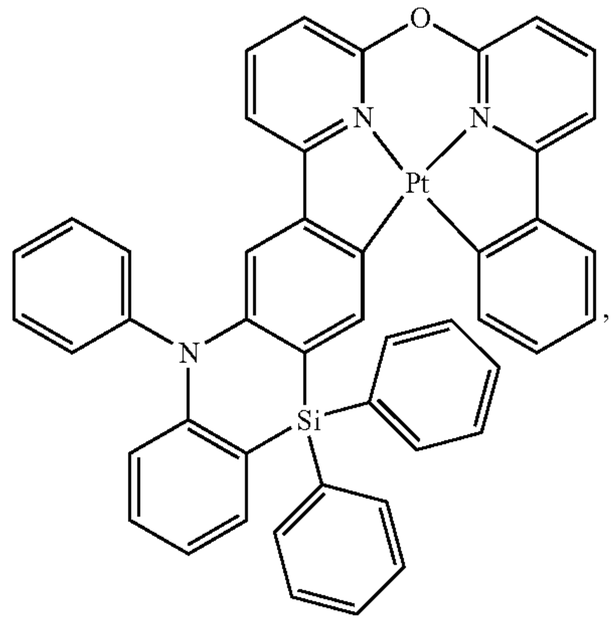
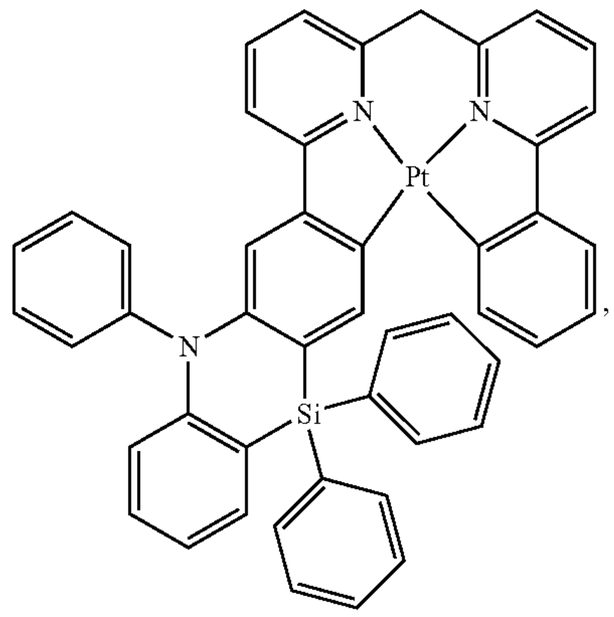
Compound 5-11



Compound 5-12



Compound 5-13

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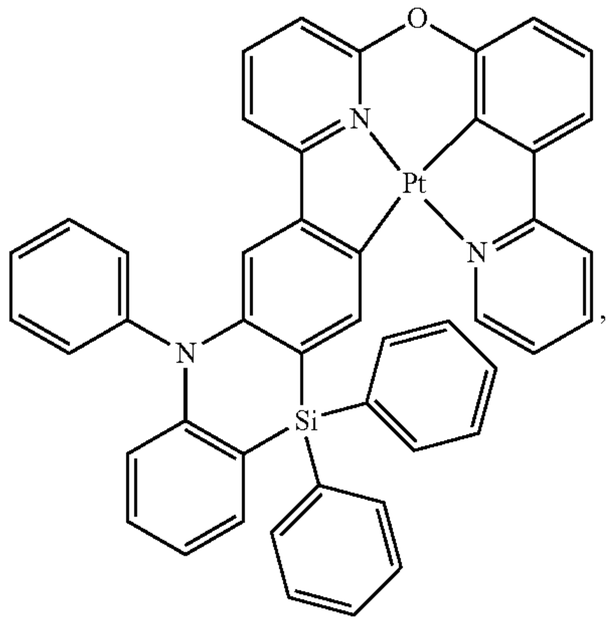
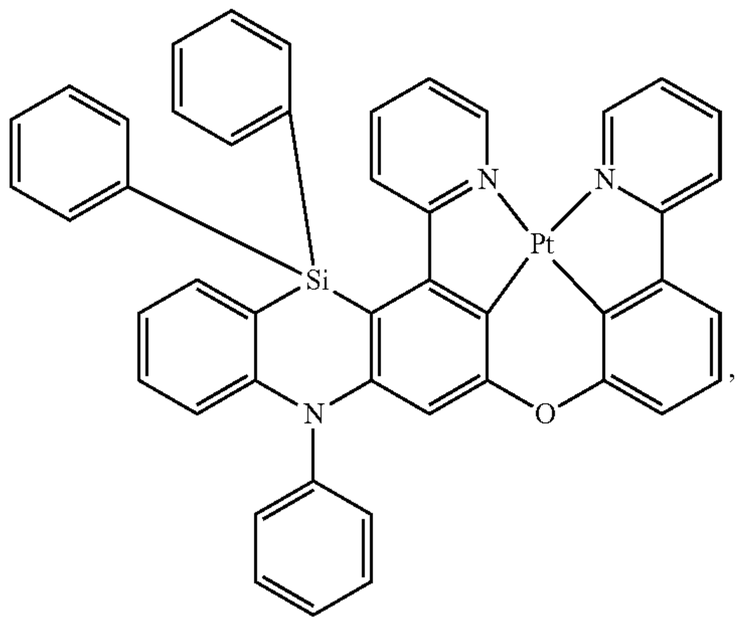
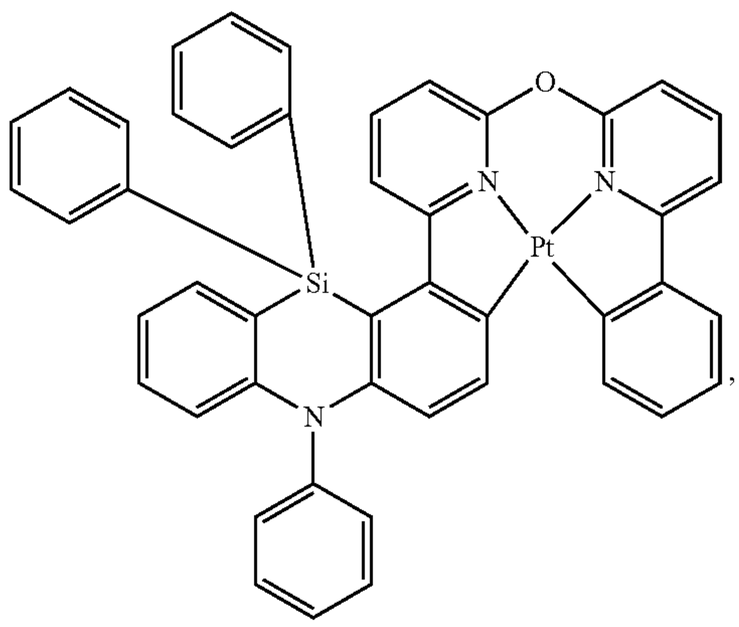
Compound 5-14



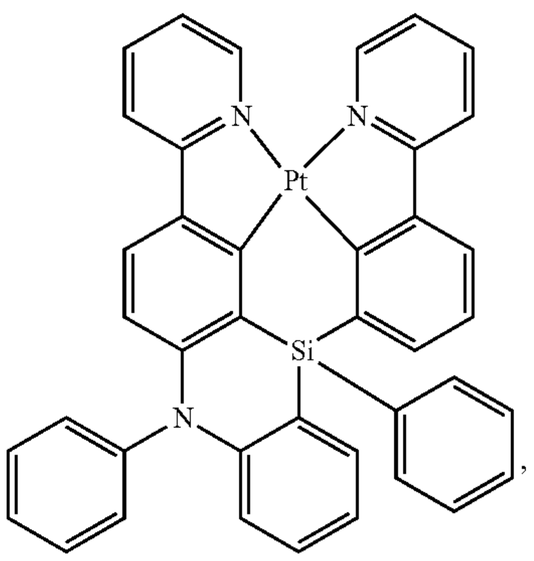
Compound 6-11



Compound 6-12



Compound 7-11



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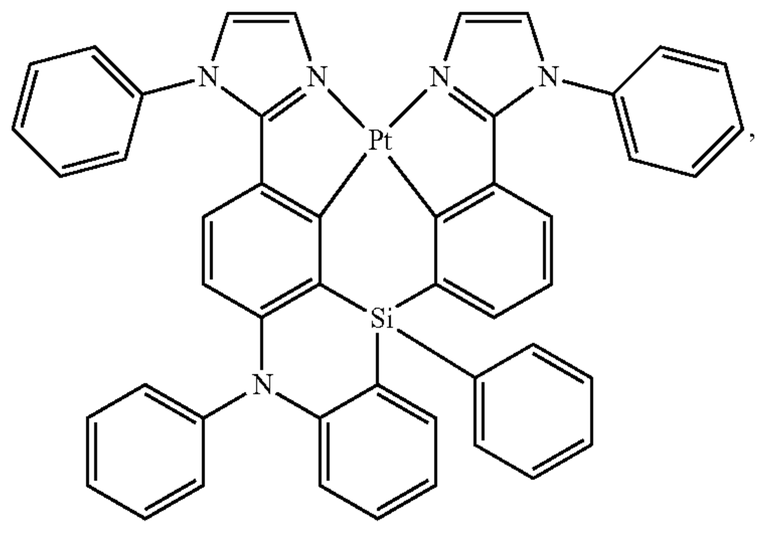
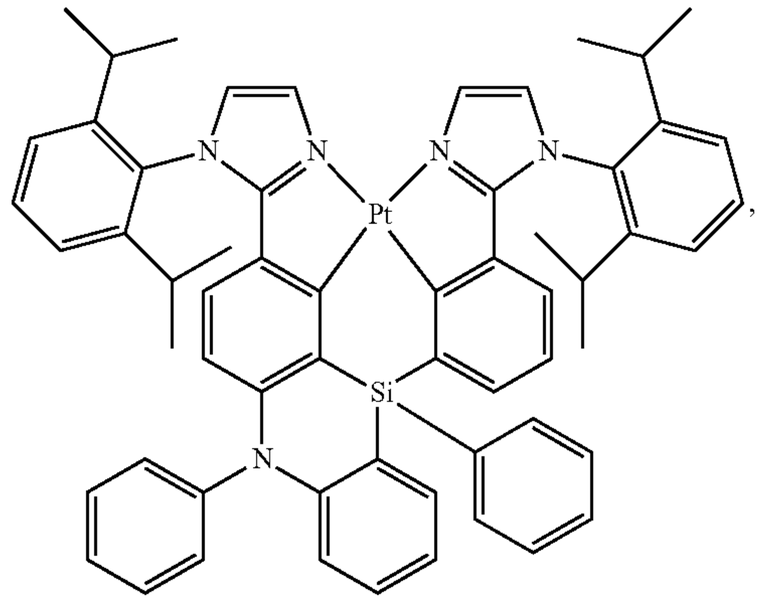
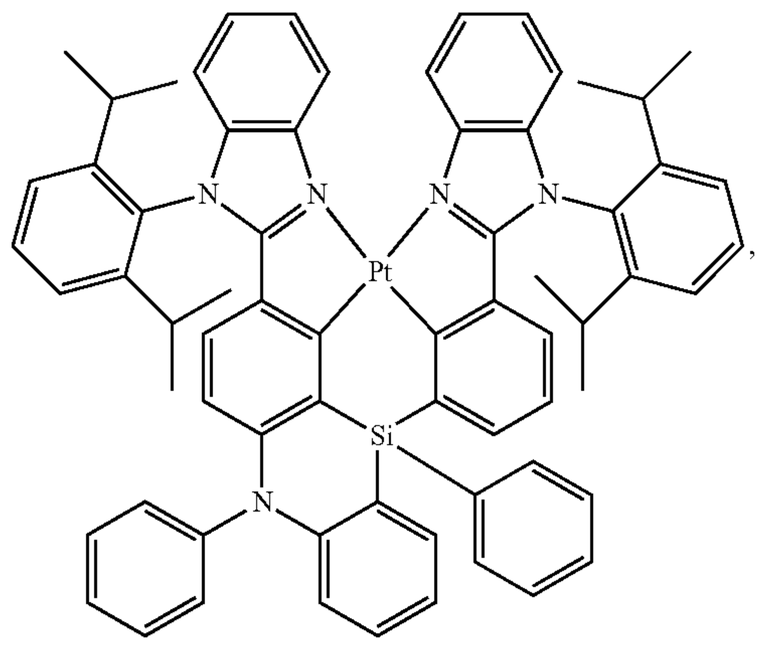
Compound 7-12



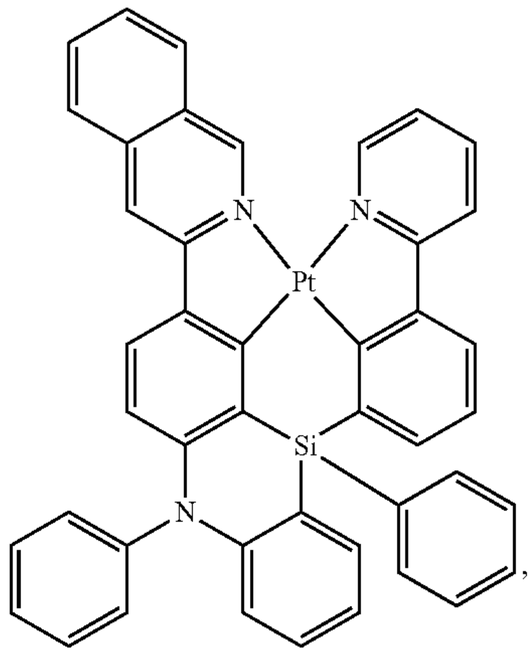
Compound 7-13



Compound 7-14



Compound 7-15



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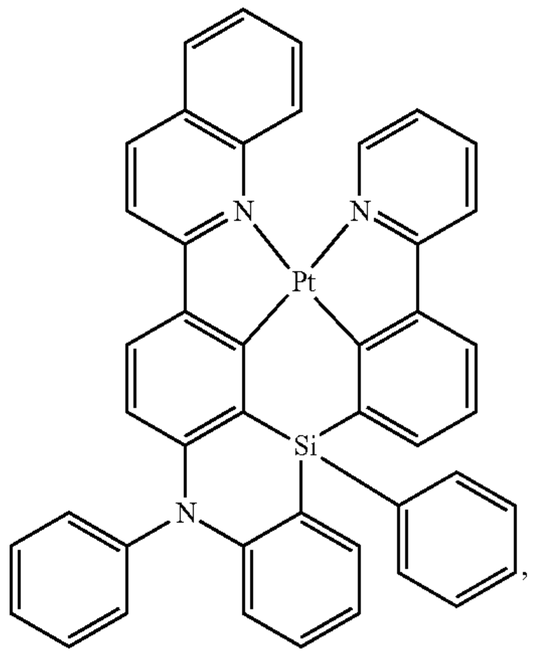
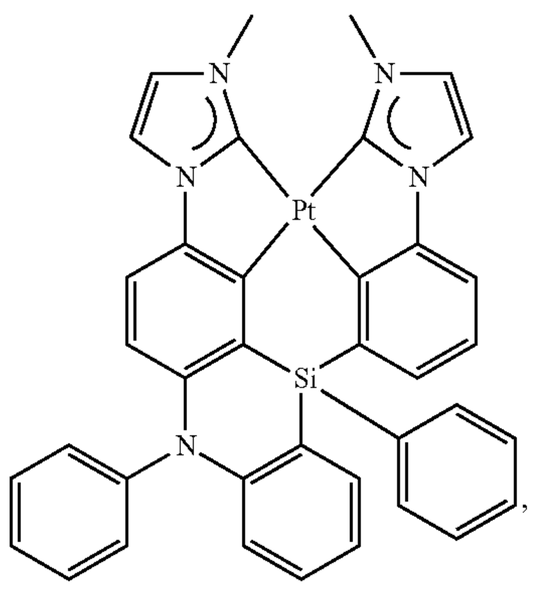
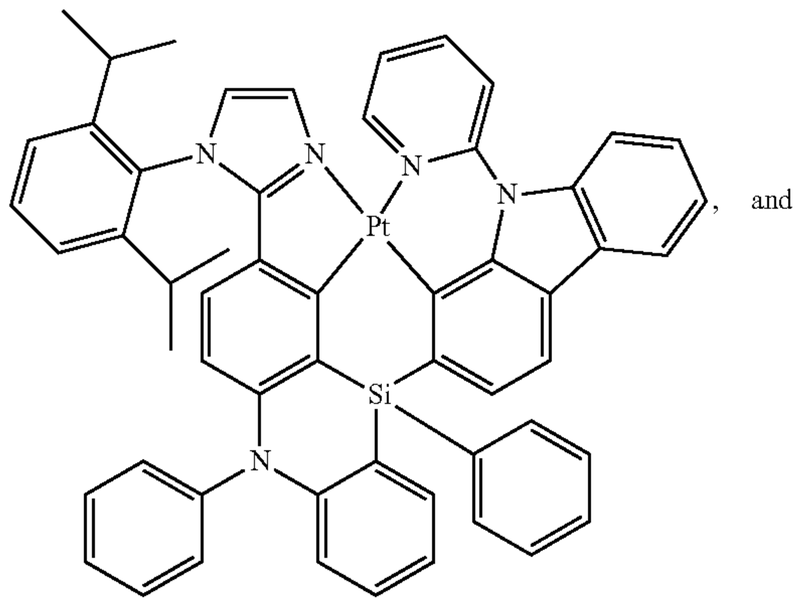
Compound 7-16



Compound 7-17

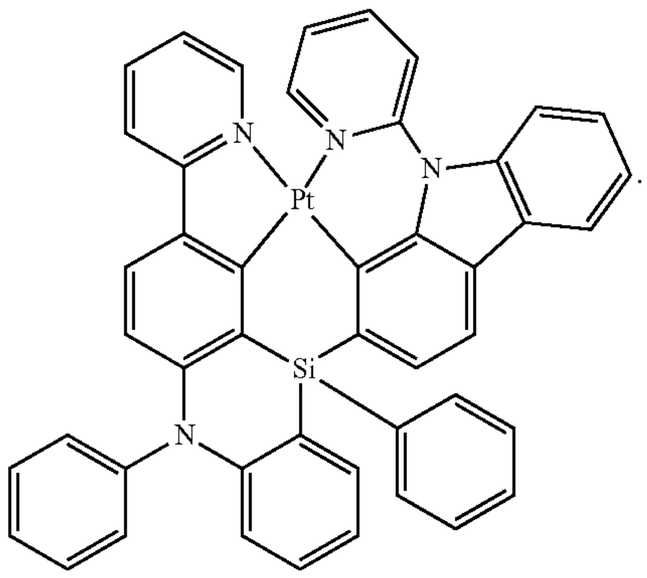


Compound 7-18



and

Compound 7-19



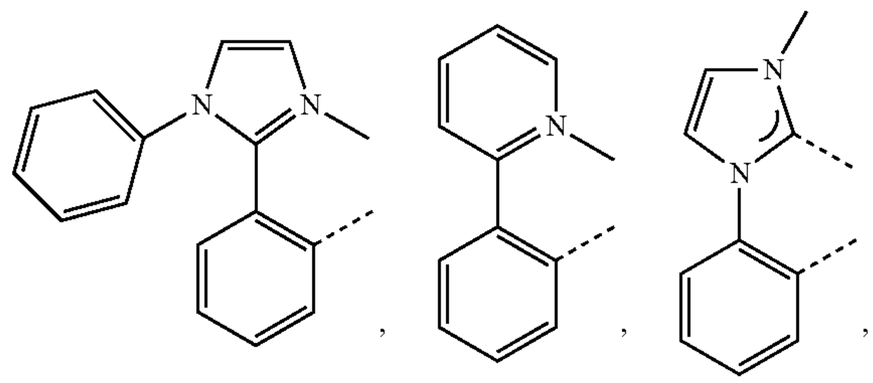
18. The compound of claim **1**, wherein R_1 comprises a 5-membered or 6-membered carbocyclic or heterocyclic aromatic ring; and

wherein R_1 is coordinated to the metal M.

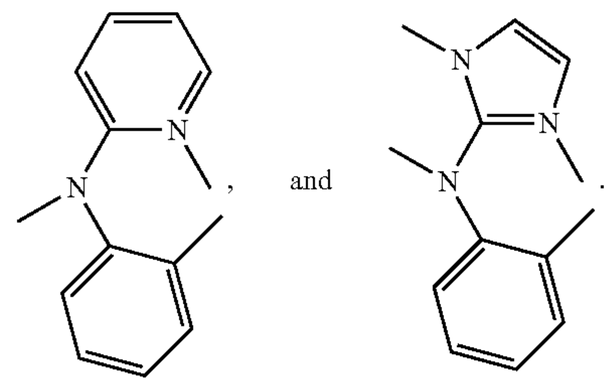
19. The compound of claim **1**, wherein R_2 comprises a 5-membered or 6-membered carbocyclic or heterocyclic aromatic ring; and

wherein R_2 is coordinated to the metal M.

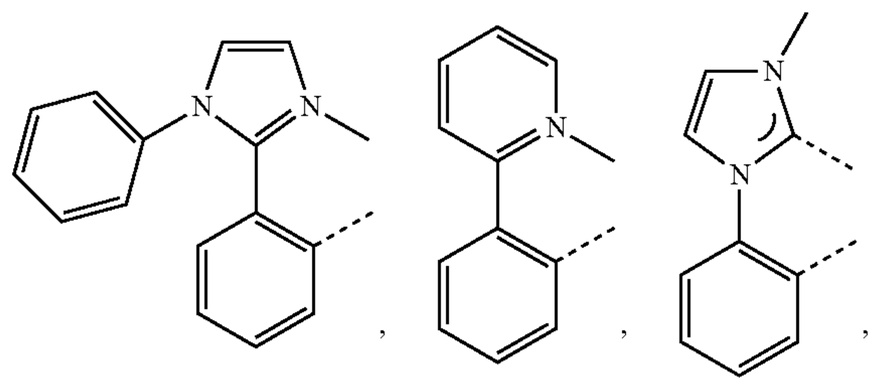
20. The compound of claim **18**, wherein R_1 comprises at least one of the chemical groups selected from the group consisting of:



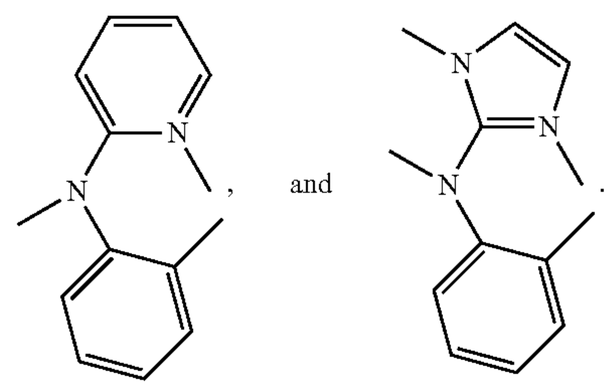
and



21. The compound of claim **19**, wherein R_2 comprises at least one of the chemical groups selected from the group consisting of:



and



22. A first device comprising a first organic light emitting device,

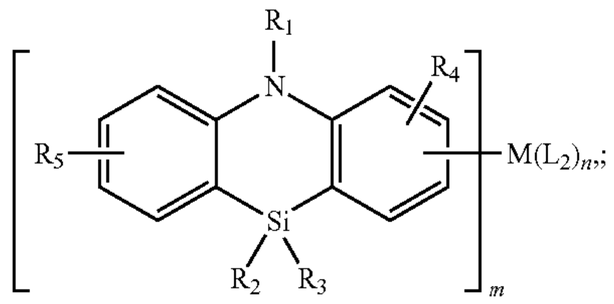
the first device comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound having a structure of Formula II:

Formula II



wherein metal M has an atomic weight higher than 40;
wherein R_5 represents mono, di, tri, tetra substitutions or no substitution;
wherein R_4 represents mono, di, or tri substitutions;
wherein each L_2 is a ligand coordinated to the metal M;
wherein each L_2 can be the same or different;
wherein R_1, R_2, R_3, R_4, and R_5 are each independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof;
wherein one R_4 is coordinated to the metal M;
wherein any two adjacent R_2, R_3, R_4, and R_5 are optionally joined to form a ring, which may be further substituted;
wherein the metal M does not form a direct bond with the N or the Si of Formula II;
wherein any of R_1, R_2, R_3, and R_4 are optionally linked to L_2 to comprise a tridentate, tetradentate, pentadentate or hexadentate ligand;
wherein m is a value from 1 to the maximum number of ligands that may be attached to the metal M; and
wherein m+n is the maximum number of ligands that may be attached to the metal M.

23. The first device of claim **22**, wherein the first device is a consumer product.

24. The first device of claim **22**, wherein the first device is an organic light-emitting device.

25. The first device of claim **22**, wherein the first device comprises a lighting panel.

26. The first device of claim **22**, wherein the organic layer is an emissive layer and the compound is an emissive dopant.

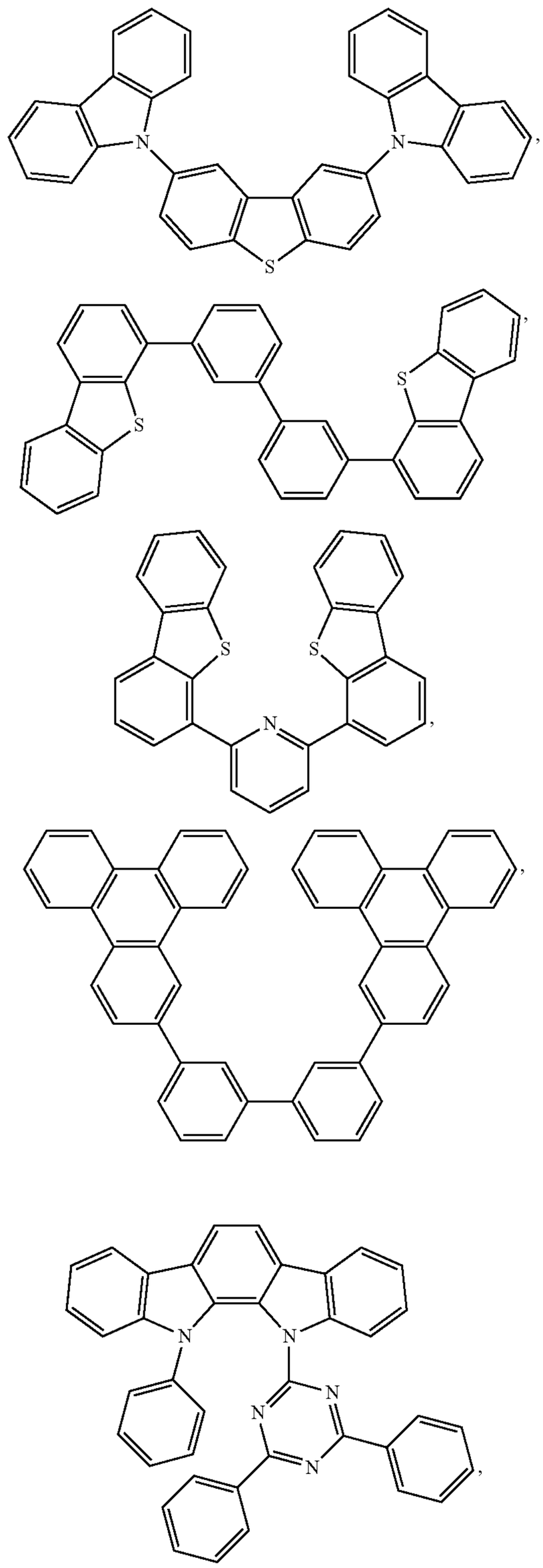
27. The first device of claim **22**, wherein the organic layer is an emissive layer and the compound is a non-emissive dopant.

28. The first device of claim **22**, wherein the organic layer further comprises a host.

29. The first device of claim **28**, wherein the host comprises a triphenylene containing benzo-fused thiophene or benzo-fused furan;
wherein any substituent in the host is an unfused substituent independently selected from the group consisting of C_nH_{2n+1}, OC_nH_{2n+1}, OAr_1, $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH{=}CH{-}C_nH_{2n+1}$, $C{\equiv}C{-}_nH_{2n+1}$, Ar_1, $Ar_t{-}Ar_2$, and $C_nH_{2n}{-}Ar_1$;
wherein n is from 1 to 10; and
wherein Ar_1 and Ar_2 are independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

30. The first device of claim **28**, wherein the host comprises at least one of the chemical groups selected from the group consisting of carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

31. The first device of claim **28**, wherein the host is selected from the group consisting of:



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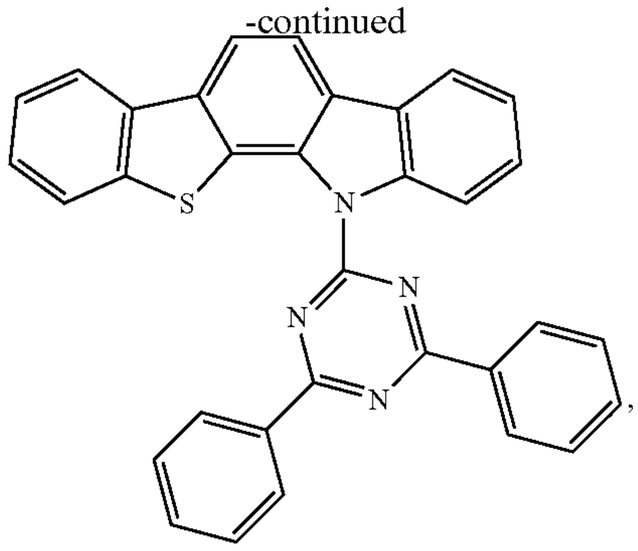

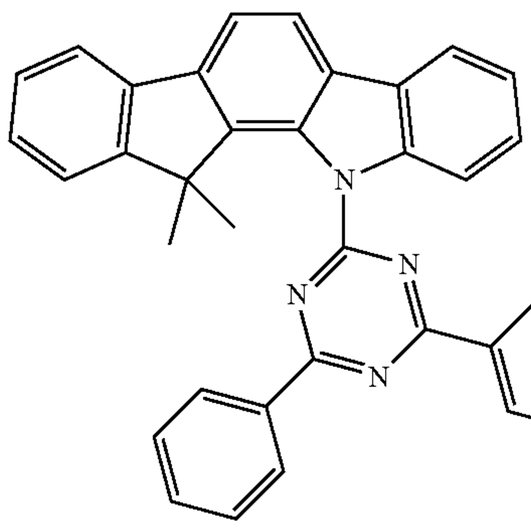

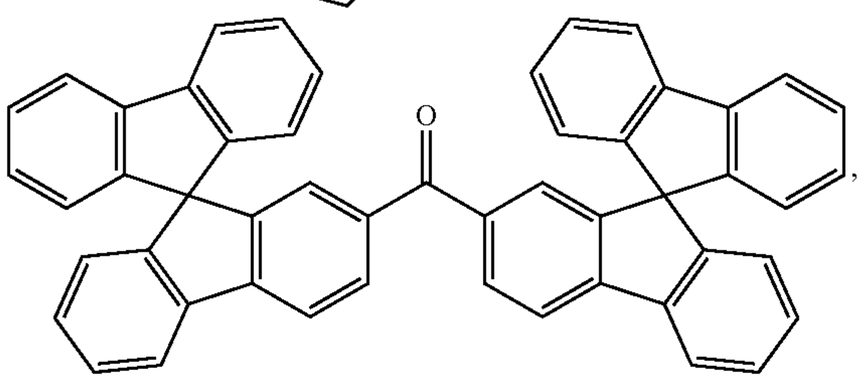

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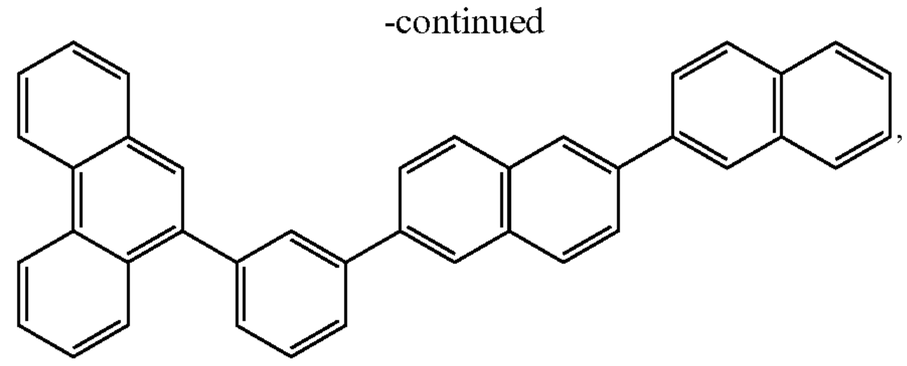
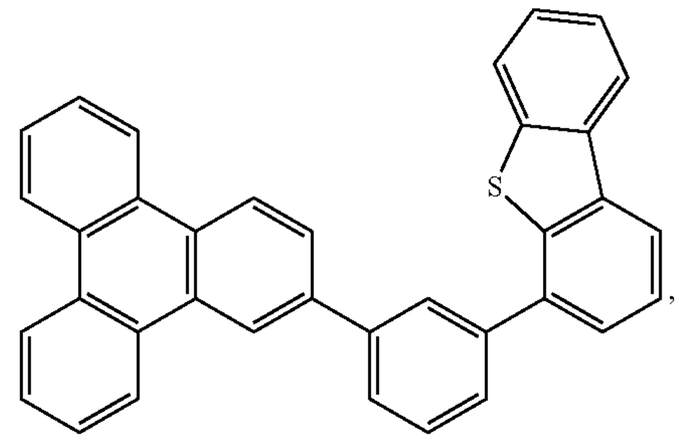
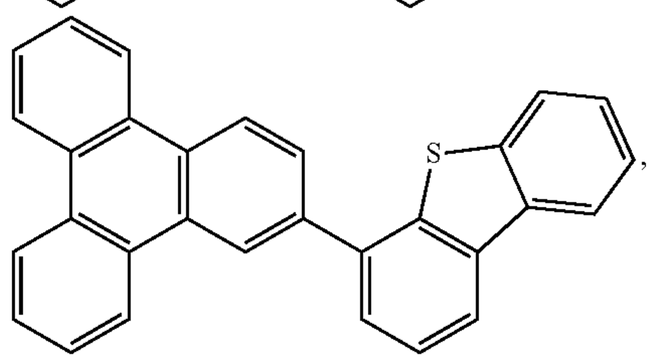






and combinations thereof.

32. The first device of claim **28**, wherein the host comprises a metal complex.

33. A formulation comprising a compound according to claim **1**.

* * * * *

UNITED STATES PATENT AND TRADEMARK OFFICE

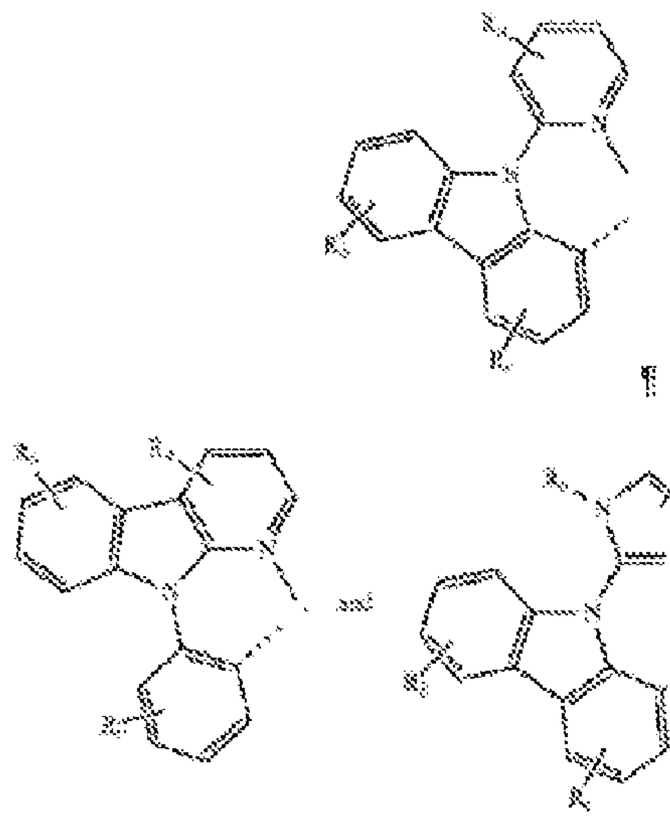
CERTIFICATE OF CORRECTION

PATENT NO. : 9,502,672 B2
APPLICATION NO. : 13/798917
DATED : November 22, 2016
INVENTOR(S) : Chun Lin et al.

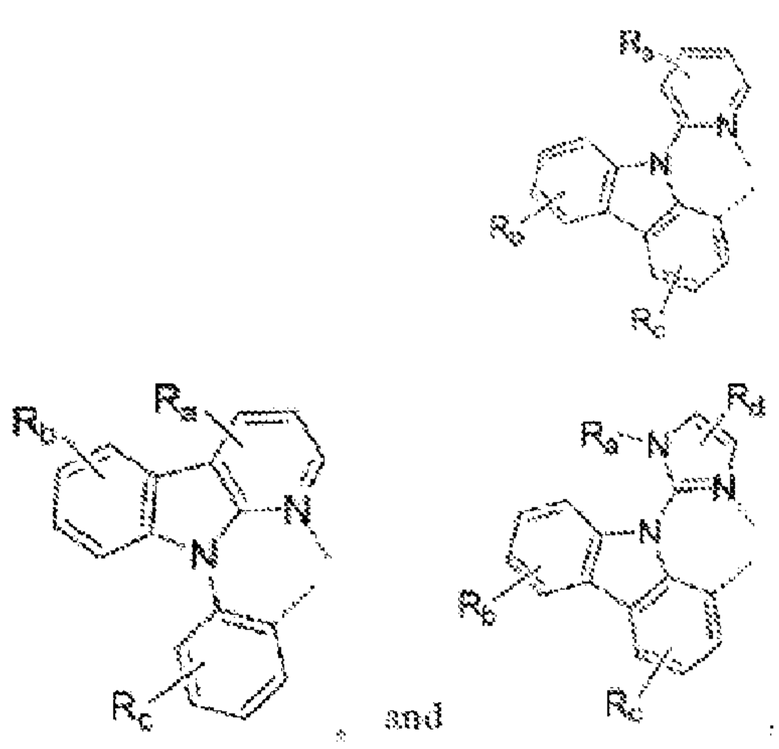
It is certified that error appears in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

In the Claims

Column 167, Lines 32-54, please delete



” and insert --



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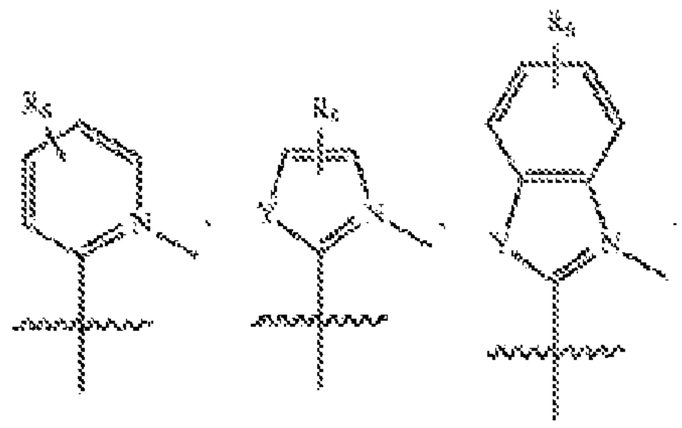
Column 169, Lines 55-67, please delete



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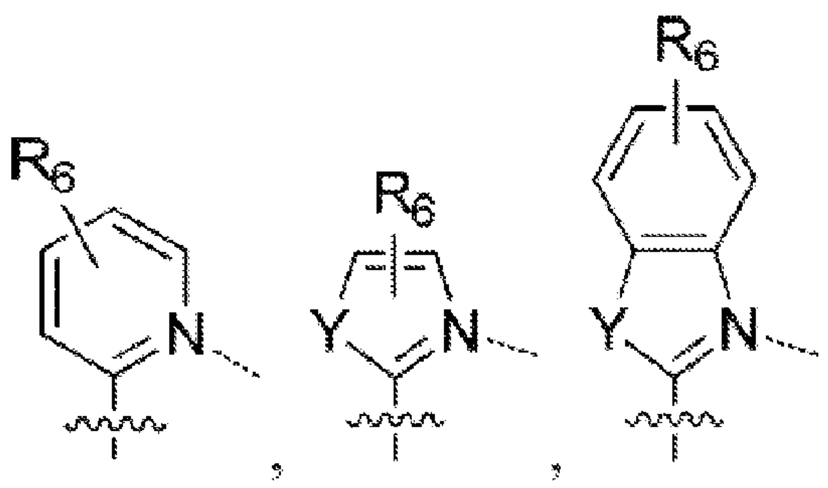

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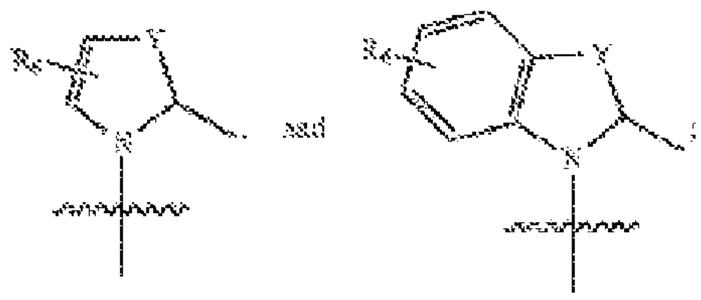
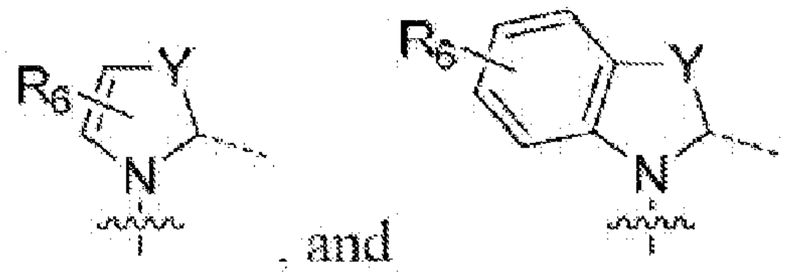
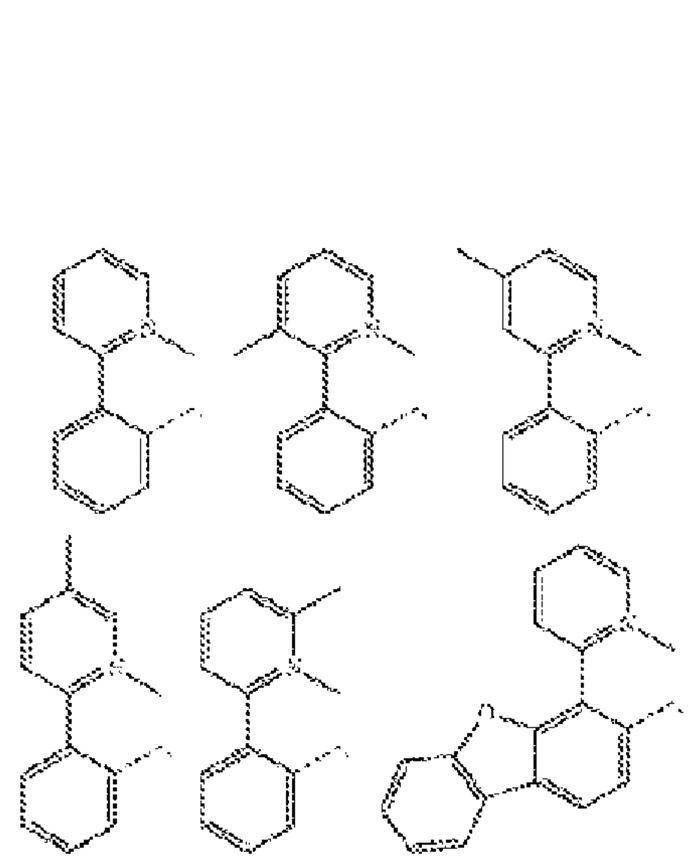
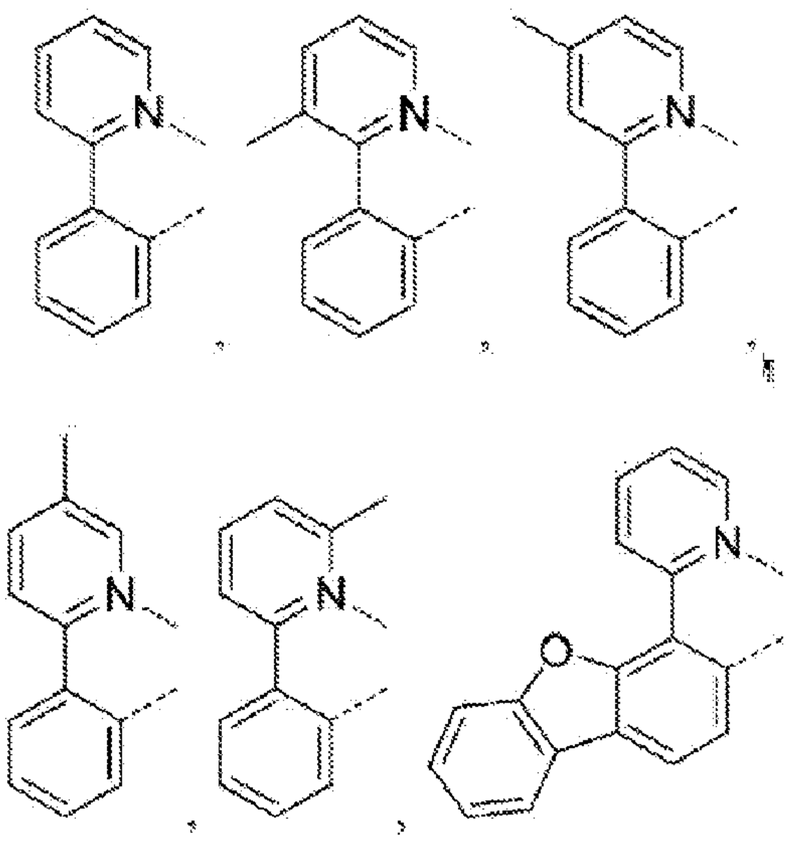
Signed and Sealed this
Twentieth Day of June, 2017

Joseph Matal
Performing the Functions and Duties of the
Under Secretary of Commerce for Intellectual Property and
Director of the United States Patent and Trademark Office

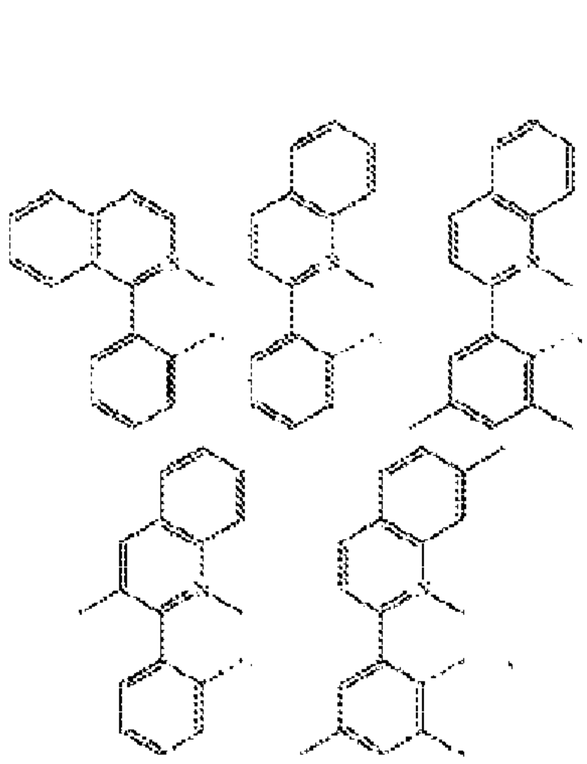
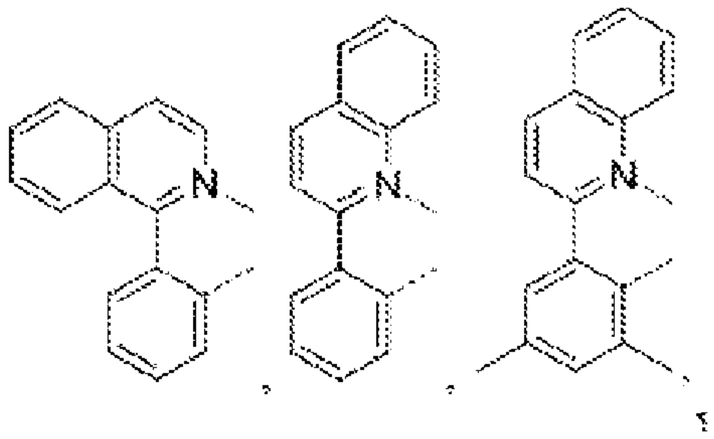
Column 170, Lines 1-10, please delete

“  ” and insert --  --

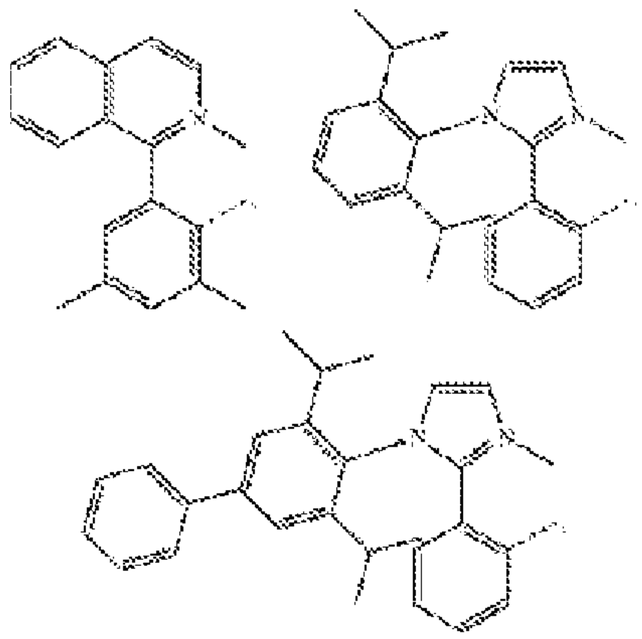
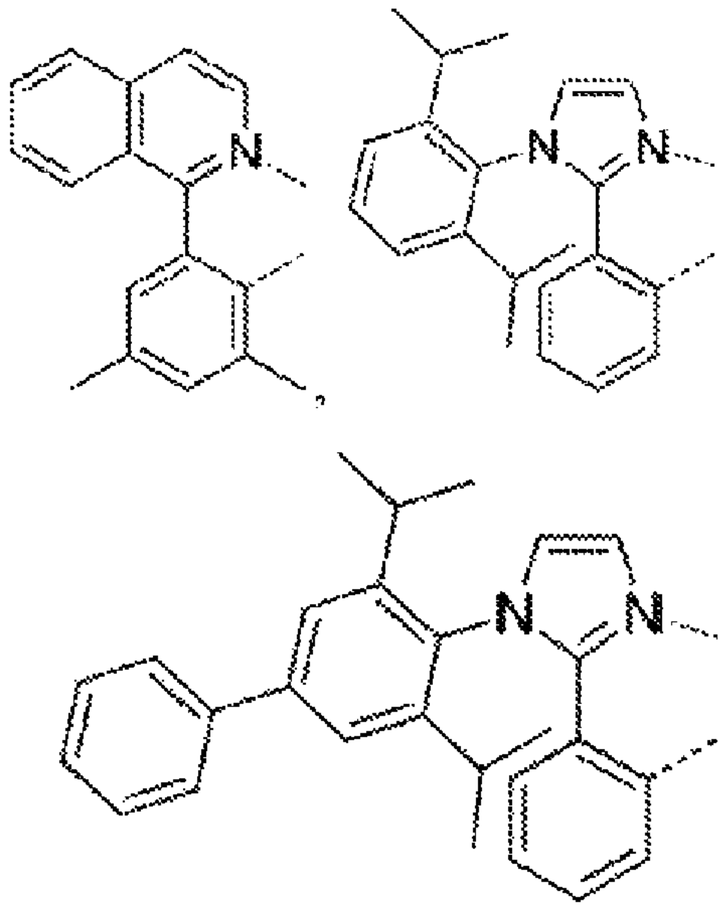
Column 175, Lines 45-67, please delete

“  ” and insert --  --

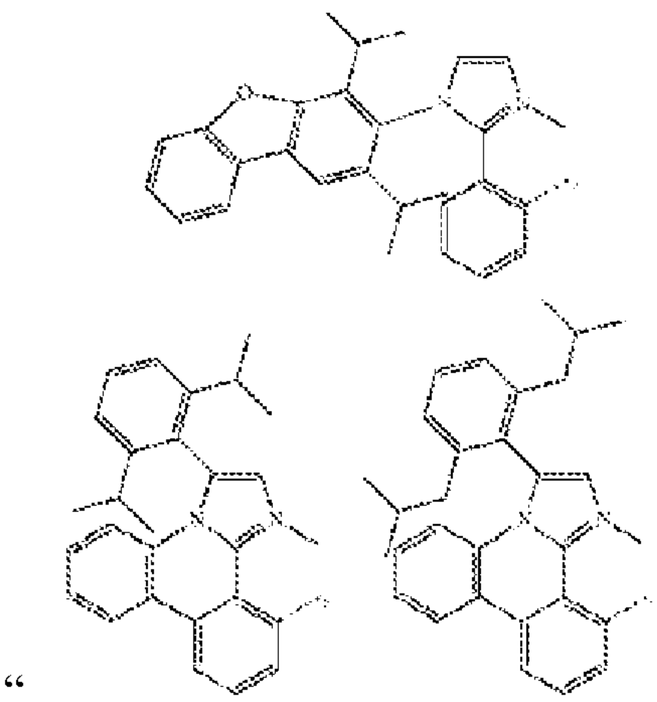
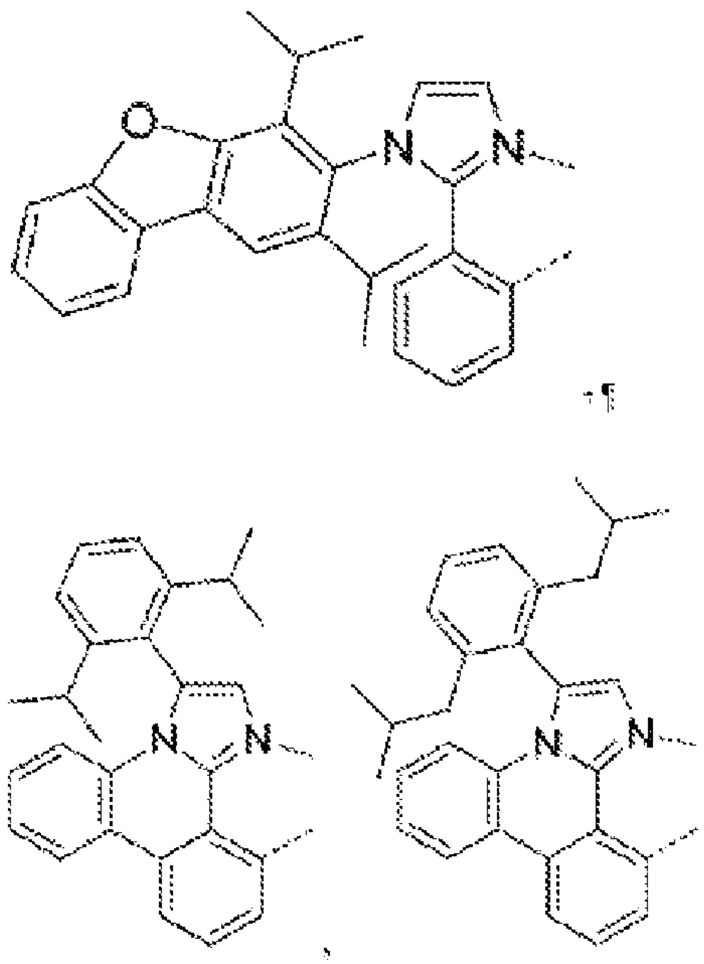
Column 176, Lines 1-24, please delete

“  ” and insert --  --

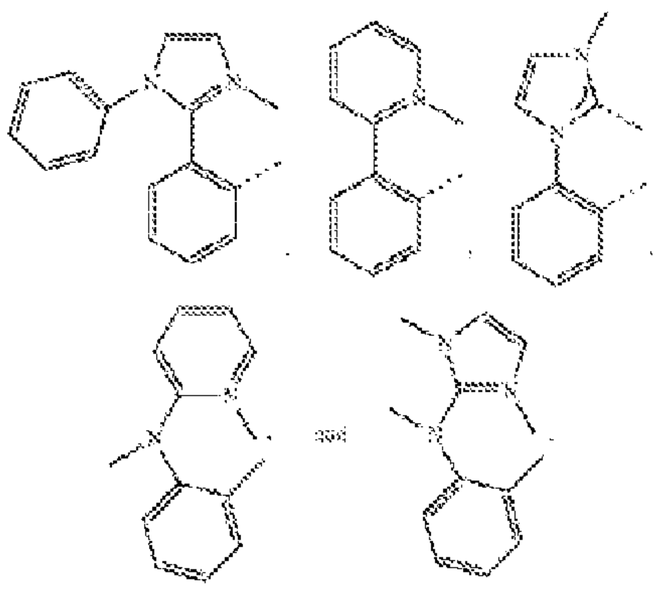
Column 176, Lines 25-42, please delete

“  ” and insert --  --

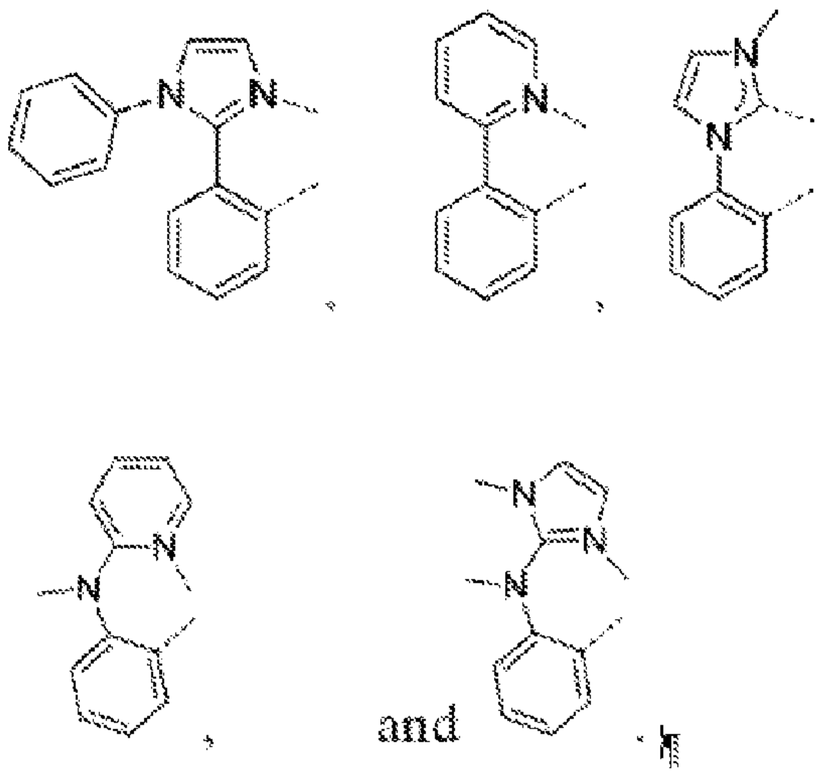
Column 176, Lines 43-67, please delete

“  ” and insert --  --

Column 186, Lines 15-35, please delete



and



“ ” and insert --

and

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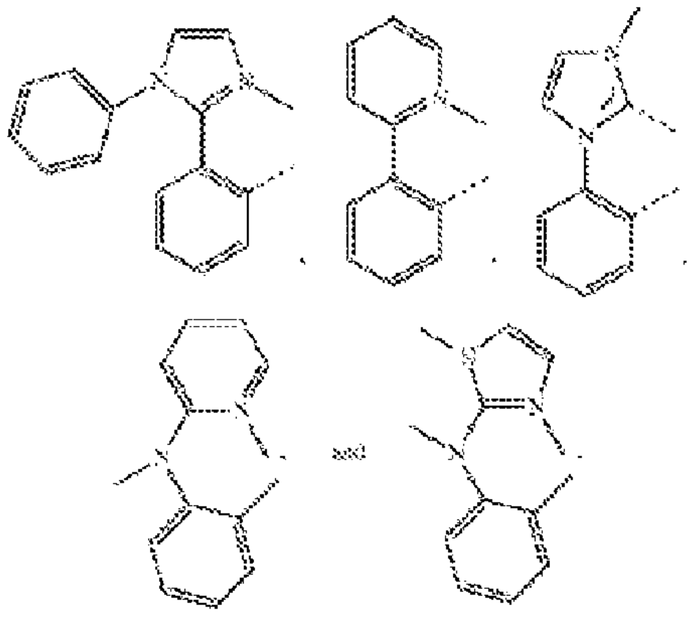
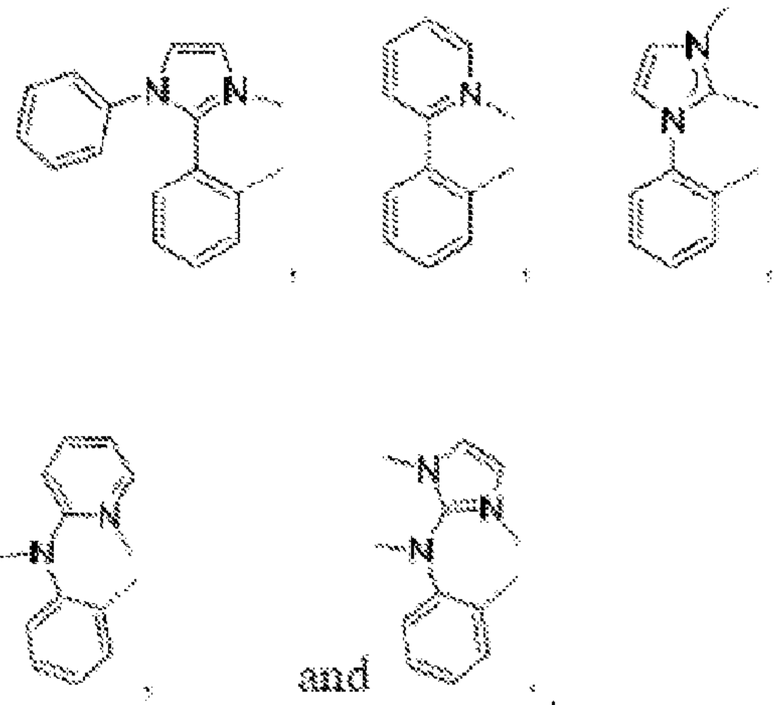
Column 186, Lines 40-60, please delete



and



“ ” and insert --

and

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